AN EXTENSIVE DATABASE OF ELECTRONIC STRUCTURE CALCULATIONS FOR COMPOUNDS BETWEEN TRANSITION METALS

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An Extensive Database of Electronic Structure Calculations for Compounds between Transition Metals

A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science at George Mason University

By

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Acknowledgments

"If you want to go fast, go alone. If you want to go far, go together." - African Proverb

It is a little known fact that I enrolled in two semesters of undergraduate physics courses before pursuing my M.Sc. in Applied Physics. It is important to highlight this because I was fortunate enough to enroll alongside the brightest group of undergraduates the Physics department had ever encountered. The countless hours spent with them in the student lounge at the whiteboard, working out problem sets and studying for exams, helped me lay a strong foundation for my future studies. To the Physics Class of 2015, I hope the world rewards you in every possible way.

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Dr. Papa is, by all accounts, the most interesting man I have ever met. His vast career spans more than four decades. He was studying and contributing to the space of DFT before it was accepted by the scientific community; before it was cool. He has met with, hosted, and befriended Nobel Laureates. He has over 200 publications to his name and is a Fellow of the American Physical Society. And even after all of this, I have only scratched the surface of his vast knowledge. The opportunity to work with Dr. Papa has been such a unique experience that I can not find a metric of comparison. All I can say is thank you. Thank you for everything, Dr. Papa.

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Abstract

AN EXTENSIVE DATABASE OF ELECTRONIC STRUCTURE CALCULATIONS FOR COMPOUNDS BETWEEN TRANSITION METALS

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Identifying materials that possess ferromagnetic or superconducting properties are of critical importance to our modern way of life. However, identifying new materials by physical experimentation is a laborious and time consuming pursuit. By leveraging advances in solid state physics and the modern computing machine, it is possible to numerically predict the fundamental properties of materials. In the field of computational materials science, Density Functional Theory (DFT) is the preferred choice for making such predictions. In this work, we apply an application of DFT, called the Augmented Plane Wave (APW) method, to predict the properties of binary compounds in the transition metal series of the periodic table. We limit the structure of these compounds to the Cesium Chloride structure and identify materials most likely to possess either ferromagnetic or superconducting properties. We perform these calculations for all possible pairs of compounds in the transition metal series, in order to explore the properties of 435 binary compounds. We use the Stoner criterion to identify materials that possess ferromagnetic properties. We use the work of McMillan and Gaspari-Gyorrfy to predict the electron-phonon coupling constant and critical temperature of materials in the superconducting state. Given the vast number of compounds we explore, all of our results are archived in our Electronic Structures

Database (ESD). Our calculations identified 63 unique compounds that meet the Stoner criterion and are likely to possess ferromagnetic properties. In particular, we predict the compound FeCd to possess large Stoner criterion greater than 5. We identified 239 compounds that satisfy our criteria for the superconducting state. We investigate those superconductors whose fundamental properties were found to be outliers of the group under study. In particular, we predict the compound ZrPd to possess a superconducting critical temperature, T_c , of $\approx 6.3K$. Additionally, we find TiNb and TiV to possess a high T_c of 21.9K and 22.2K, respectively. Further calculations will need to be performed to determine the ground state structure and stability of the 435 compounds explored in this work.

Chapter 1: Introduction

Materials that possess magnetic or superconducting properties are of critical importance to our modern way of life. Applications such as electric motors, digital storage, medical devices, and even particle accelerators, to name a few, are based on materials that possess either magnetic or superconducting properties. One interesting application space is in magnetic refrigeration, which is based upon the magnetocaloric effect, in which a materials temperature can be changed by exposing it to changing magnetic field. The magnetocaloric effect can be enhanced by using a magnet with a small heat capacity and a large magnetic field. Leveraging this effect is also useful for cooling materials to their critical temperature, when the material achieves a superconducting state. But superconductors that require ultra cold environments are difficult to apply outside a laboratory setting. Identifying materials with a high critical temperature would yield more types of applications. Applications such as enhanced transmission lines for power distribution. Our quest to create better machines starts with better materials. However, the process of identifying new materials that possess the requisite properties by physical experimentation is a laborious and time consuming pursuit. Alternatively, it is possible to leverage advances in solid state physics, coupled with the modern computing machine, to numerically predict the fundamental properties of materials. These numerical predictions serve to complement and guide the experimenter to discover novel and new materials. In the field of computational materials science, Density Functional Theory (DFT) is the preferred choice to predict the fundamental properties of materials. Currently, there are many variations and expansions of DFT to choose from. In this work, we use the Muffin-Tin (MT) form of the Augmented Plane Wave (APW) method of DFT to calculate the fundamental properties of binary compounds in the transition metals series. We limit the structure of these compounds to the Cesium-Chloride (CsCl, or B2) structure and identify materials most likely to possess either ferromagnetic or superconducting properties. Additionally, we compare aspects of our results against alternative numerical methods, such the Generalized Gradient Approximation (GGA), the Linearized Augmented Plane Wave (LAPW) method, and the Tight-Binding (TB) method.

Magnetism occurs due to the motion of an electron orbiting a nucleus and the spin of the electron about its axis. The orbital and spin motion impart a magnetic moment upon the electron, creating a tiny magnet. Thus, magnetism is a macroscopic observation generated by a microscopic quantum mechanical effect due to the fundamental magnetic dipole moment of an electron and the Pauli exclusion principle. The quantum nature of electrons dictates that its spin can be in only one of two states, "up" or "down"; then the magnetic field can only be "up" or "down". When the individual fields are aligned in the same state, the cumulative macroscopic effect is the observed magnetic field. However, the Pauli exclusion principle states that two identical electrons cannot occupy the same quantum state simultaneously. Therefore, elements whose electron shells are filled will have total magnetic dipole moment of zero, because one state will cancel its opposing state. Only elements with partially filled shells possess a magnetic property. This gives rise to the different types of observed magnetic behavior: paramagnetic, ferromagnetic, antiferromagnetic, and ferrimagnetic. The focus of this work is on ferromagnetic behavior, in which the magnetic dipole moments are aligned in the same state.

Superconductivity is another phenomenon possessed by certain materials that when cooled below a particular critical temperature, the material has an electric resistance of exactly zero and no observable magnetic field. Superconductivity was first observed in 1911 by Dutch physicist Heike Kamerlingh Onnes [1], in which he cooled mercury to 4 degrees Kelvin and the resistance disappeared. Explaining this phenomena is an active area of study, but a widely accepted criteria for superconductivity is grounded in the Bardeen-Cooper-Schrieffer [2] (BCS) theory that relates the interaction of electrons with lattice vibrations, known as electron-phonon interactions. In a conductor, an electric field causes free electrons to move within the lattice structure. As electrons flow within the lattice, they collide with their neighbors causing resistance to the flow of electrons. Moving electrons attract positive charges in the lattice, causing the lattice to slightly deform. This deformation, called a phonon, causes another electron with opposite spin to occupy the region of higher positive charge density. Now the movement of two electrons are correlated with each other, creating a Cooper pair. As more of these Cooper pairs form, fewer collisions occur, causing the resistance to go to zero. In the superconducting state, the magnetic field of the surface current will cancel the magnetic field within the bulk of the material, such that the measured magnetic flux is zero. This behavior is called the Meissner effect, after German physicist Walther Meissner observed the phenomena in 1933 [3]. This work uses BCS theory to model electron interactions within a lattice to predict fundamental superconductor properties, such as the electron-phonon interaction and the critical temperature.

The phenomena of ferromagnetism and superconductivity are explained by the motion and interaction of electrons within a material. A widely accepted model of electronic behavior is the Schrödinger equation. DFT is a method for solving the many-body Schrödinger equation by expressing the electron density as a functional in terms of the wave function. The APW method of DFT is based in the muffin-tin approximation, in which the wave function describing the potential field is assumed to be spherically symmetric within the region of the muffin-tin, and constant outside the region. The muffin-tin approximation is convenient in that it allows us to model the wave function in terms of the well known radial form of Schrödingers equation. We apply the APW method of DFT to calculate the ground state energy, the equilibrium lattice constant, the electronic band structure, the density of states (DOS), the Fermi energy level, and the DOS at the Fermi energy level. In order to predict whether or not a material possesses ferromagnetic behavior, we calculate the Stoner criterion [4]. We use the work developed by McMillan [5] to determine the electron-phonon coupling constant and the superconducting critical temperature.

At the time that methods such as the APW were introduced, computational power was limited and the time to execute these methods was considerable. Advancements in computing, most notably the strength of the modern CPU, allows us to execute these methods in remarkably less time. Instead of exploring a handful of compounds, we are now able to explore hundreds, even thousands, of compounds in very short order. A given compound can be described by a myriad of properties, and our calculations allow us to explore or add to this set of known properties. This explosion of data in materials science, as well as other fields, has created new challenges, and a new area of study commonly referred to as Big Data. We facilitate this new field by archiving all of our results in a database that we call the Electronic Structures Database (ESD).

In this work, we present our predictions for diatomic compounds within the transition metal series that possess either ferromagnetic or superconducting properties. All calculations are performed on compounds in the CsCl configuration. Where possible, we compare with experiment or similar calculations. In total, 435 compounds were investigated, of which 60 are known to be thermodynamically stable in the CsCl configuration. Given the large number of compounds investigated, this work can be viewed as existing at the intersection of materials science and Big Data. Of the 435 compounds investigated, we find 63 compounds that possess a ferromagnetic property, and 239 compounds that possess a possible superconducting state. However, it has been established that a material cannot be both ferromagnetic and superconducting at exactly the same composition. Compounds that satisfy both ferromagnetic and superconducting criteria are eliminated as possible superconductors. The results of all calculations performed in this work are archived in our publicly available database, which can be found at http://esd.spacs.gmu.edu/db/.

In Chapter 2 we will expand on the theory behind the MT-APW method along with an introduction to crystallography and the definition of reciprocal space. We conclude Chapter 2 with a brief discussion of numerical implementation of the MT-APW method and our process for executing such an implementation. In Chapter 3 we will discuss the contents and usage of the ESD. In Chapter 4, we present our findings for ferromagnetic and super-conducting properties. We provide a focused discussion of materials whose ferromagnetic or superconducting properties are found to be unique outliers. In Chapter 5, we will discuss ways in which this work can be expanded.

Chapter 2: Theory and Methods

2.1 Density Functional Theory, the Muffin-Tin Approximation, and the Augmented Plane Wave

Our purpose is to identify materials that may possess either ferromagnetic or superconducting properties. We know that ferromagnetism is due to the spin alignment of electrons. Additionally, superconductivity can be explained by the electron-phonon interaction described by BCS theory. Both properties depend upon our understanding of the behavior of electrons. The most common model used to describe the dynamics of electrons is the Schrödinger equation. However, the Schrödinger equation in its simplest form is suitable for hydrogen-like systems only. Most materials are more complex, and we must use methods capable of solving many-electron systems. Building on the Schrödinger equation, we can apply techniques from variational calculus to devise a system of equations to approximate the electron states of a system. The most commonly used of such approximation methods is Density Functional Theory (DFT), developed by Kohn, Hohenberg, and Sham, [6,7] for which Kohn was the awarded 1998 Nobel Prize in Chemistry. In the following sections, we will describe the foundations of DFT and its extensions employed to predict materials that possess either ferromagnetic or superconducting properties.

The single-electron Schrödinger equation is stated as

$$\left[-\frac{\hbar}{2m}\nabla^2 + V(r)\right]\psi(r) = \epsilon\psi(r)$$
(2.1)

where the first term is the kinetic energy, V is the potential energy, ψ is the wavefunction, and ϵ is the total energy. DFT expands on equation 2.1 by the approximating the total energy, E, as a functional of the ground state electronic density, ρ , where ρ is the density that minimizes $E(\rho)$.

The key insight of DFT is that the total energy can be described entirely by the electron density for each electron in the system, thereby reducing an intractable many-electron problem to a tractable single-electron problem. By DFT, the total energy of the system is expressed as

$$E(\rho) = E_h(\rho) + E_{xc}(\rho) \tag{2.2}$$

where E_h is the Hartree energy, expanded as

$$E_h(\rho) = T(\rho) + E_{e-e}(\rho) + E_{e-n}(\rho) + E_{n-n}(\rho)$$
(2.3)

where T is the single particle kinetic energy, E_{e-e} is the Coulomb interaction between electrons, E_{e-n} is the interaction energy between electrons and nuclei, and E_{n-n} is the interaction energy between nuclei. The E_{xc} term is the energy exchange and correlation term, which is not explicitly defined by DFT, but is given by

$$E_{xc}(\rho) = \int \rho(r)\epsilon_{xc}(\rho)d^3r \qquad (2.4)$$

where ϵ_{xc} is approximated by a fit to the energy of a uniform electron gas. Having defined the total energy as function of the electron density, the minimization of $E(\rho)$ yields a *set* of single-electron Schrödinger equations to solve, re-written as

$$\left[\frac{-\hbar}{2m}\nabla_i^2 + V(r)\right]\psi_i(r) = \epsilon_i\psi(r)$$
(2.5)

where V(r) is the sum of the Coulomb potential, V_c , with the exchange and correlation potential, V_{xc} . We will return to discuss the exchange and correlation terms. To find V(r), we solve Poisson's equation that relates $\rho(r)$ to the Coulomb potential, $V_c(r)$, by the relationship

$$\nabla^2 V_c(r) = 8\pi\rho(r) \tag{2.6}$$

where the charge density, $\rho(r)$ is the summation over the occupied states, $\sum_i \psi_i^2$.

The exchange and correlation term in equation 2.2 is intended to incorporate the remaining physics not captured by the obvious particle interactions described by the Hartree energy in equation 2.3. The concept of exchange is a representation of the Pauli Exclusion principle, which states that two identical electrons cannot occupy the same quantum state simultaneously. Stated another way, if the positions of two electrons are exchanged, then the total wavefunction changes sign, thereby demonstrating the requirement that the exchange energy must be anti-symmetric, which is expressed as

$$E_X = -\int \int \psi_i(r_1)\psi_j(r_2) \frac{1}{r_{12}}\psi_i(r_2)\psi_j(r_1)dr_1dr_2$$
(2.7)

and we note the exchange of position between ψ_i and ψ_j . However, the concept of correlation is not as clearly defined, but is typically defined as the difference between the many-body quantum mechanics result and the Hartree-Fock result. Nonetheless, developing an appropriate model of the exchange and correlation term is an area of active study, providing trade-offs between different models.

Within the scope of this work, we define the exchange and correlation term by the Local Density Approximation (LDA) method [8]. Specifically, we use a form of the LDA known as the $X\alpha$ method [9]. In the $X\alpha$ method, the exchange potential is define as

$$V_x(r) = \alpha \left(\frac{3\rho(r)}{8\pi}\right)^{1/3} \tag{2.8}$$

where α is a coefficient that is varied between 2/3 and 1 to agree with the Hartree-Fock total energy. The exchange and correlation term, $V_{xc}(r)$, uses the form proposed by Hedin and Lundqvist [10], given as

$$V_{xc}(r) = \alpha \beta(r_s) \left(\frac{3\rho(r)}{8\pi}\right)^{1/3}$$
(2.9)

where $\alpha = 2/3$ is the Kohn-Sham parameter and β is the correlation enhancement factor defined as

$$\beta(r_s) = 1 + B \ln\left(1 + \frac{1}{x}\right) \tag{2.10}$$

where $r_s = (3/4\pi\rho(r))^{1/3}$, $x = r_s/21$, and B = 0.7734.

Up to this point, we have described the foundations of DFT and our use of the LDA method to define the exchange and correlation term. However, while we have presented a model for the energies in the system, we must also have a model for the wavefunction. We stated earlier that the electron density is expressed as the sum over the occupied states. The occupied states are captured in the definition of the wavefunction, which are the atomic orbitals. It is typical to model the atomic orbitals as a sum of Gaussian functions, such that

$$\psi(\mathbf{r}) = \sum_{j=1}^{N} d_j \phi_j^{GF}(\mathbf{r})$$
(2.11)

where N is the number of Gaussian orbitals used, ϕ_j is the atomic orbital, and d_j are the coefficients. The choice of model for ϕ_j is another distinction between methods. In this work, we use the Muffin-Tin Augmented Plane Wave (MT-APW) method, originally proposed by Slater in 1937 [11]. In the MT approximation, each atomic site is surrounded by a sphere, much like the tins used to bake muffins, and hence the name "muffin-tin". Outside of the sphere, the interstitial region, where the potential is assumed to be a constant V_c , the wavefunction is modeled as a plane wave,

$$\phi(\mathbf{r}) = \exp(i\mathbf{k} \cdot \mathbf{r}) \tag{2.12}$$

Inside the muffin-tin sphere, where the potential is assumed to be spherically symmetric, the wavefunction has the form of spherical harmonics, $Y_{\ell m}$,

$$\phi(\mathbf{r}) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} A_{\ell m} Y_{\ell m} u_{\ell}(\mathbf{r}, \epsilon)$$
(2.13)

where $A_{\ell m}$ is chosen such that equations 2.12 and 2.13 are continuous at the boundary of the sphere of radius R_n . The u_ℓ term is the radial wavefunction of the Schrödinger equation, i.e.

$$-\frac{1}{2r^2}\frac{d}{dr}\left(r^2\frac{du_{\ell}(r)}{dr}\right) + \left(\frac{\ell(\ell+1)}{r^2} + V(r) - \epsilon_{\ell}\right)u_{\ell}(r) = 0$$
(2.14)

where V(r) is found by solving Poisson's equation, and the $Y_{\ell m}$ term are the Legendre polynomials,

$$Y_{\ell m} = P_{\ell}^{|m|}(\cos\theta) \exp(im\phi)$$
(2.15)

Since V(r) is a periodic function, the wavefunction satisfies the Bloch condition [12],

$$\Psi(r+G_n,k) = \exp(ikG_n)\Psi(r,k) \tag{2.16}$$

Substituting equation 2.16 into equation 2.5 yields a system of N algebraic equations

$$\sum_{j=1}^{N} (H - \epsilon)_{ij} C_{kj} = 0$$
(2.17)

which is a familiar eigenvalue problem, where ϵ is the energy. The eigenvalues that yield a determinant that is equal to zero are the energy states of the system. Solving equation 2.17 allows us to calculate the ground state energy from first-principles.

2.2 Crystal Structure and Brillouin Zones

Atomic elements that take on a solid phase will exist as a collection in a particular three dimensional crystal structure, the most common of which are shown in Figure 2.1.



Figure 2.1: Common crystal structures: Simple Cubic (SC), Body Centered Cubic (BCC), Face Centered Cubic (FCC), and Hexagonal Close Packed (HCP)

It is when we consider atoms to exist in a crystal structure that we can investigate the properties of materials, using the Schrödinger equation as our primary tool. Each crystal structure has a particular geometry that determines the behavior of the electron. A crystal is described in real space in terms of the primitive lattice vectors \vec{a}_1 , \vec{a}_2 , \vec{a}_3 , and the positions of the atoms inside the primitive cell are described by the Bravais lattice vector, $\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$. The primitive cell is defined as the volume, Ω , enclosed by the three primitive vectors,

	sc	bcc	fcc	diam	hcp
Conventional Cell Volume	a^3	a^3	a^3	a^3	$\frac{3\sqrt{3}}{2}a^2c$
Lattice points per cell	1	2	4	4	6
Primitive Cell Volume	a^3	$\frac{a^3}{2}$	$\frac{a^3}{4}$	$\frac{a^3}{4}$	$\frac{\sqrt{3}}{2}a^2c$
Packing Fraction	$\frac{1}{6}\pi$	$\frac{\sqrt{3}}{8}\pi$	$\frac{\sqrt{2}}{6}\pi$	$\frac{\sqrt{3}}{16}\pi$	$\frac{\sqrt{2}}{6}\pi$

Table 2.1: Basic properties of common crystal structures. [13]

$$\Omega = |\vec{a}_1(\vec{a}_2 \times \vec{a}_3)| = \begin{vmatrix} a_{1x} & a_{1y} & a_{1z} \\ a_{2x} & a_{2y} & a_{2z} \\ a_{3x} & a_{3y} & a_{3z} \end{vmatrix}$$
(2.18)

The behavior of electrons in a crystal is based on the concept of the reciprocal lattice. The primitive lattice vectors in reciprocal space are defined by

$$\vec{b}_1 = \frac{2\pi(\vec{a}_2 \times \vec{a}_3)}{\vec{a}_1(\vec{a}_2 \times \vec{a}_3)} \tag{2.19}$$

$$\vec{b}_2 = \frac{2\pi(\vec{a}_3 \times \vec{a}_1)}{\vec{a}_2(\vec{a}_3 \times \vec{a}_1)} \tag{2.20}$$

$$\vec{b}_3 = \frac{2\pi(\vec{a}_1 \times \vec{a}_2)}{\vec{a}_3(\vec{a}_1 \times \vec{a}_2)} \tag{2.21}$$

The lattice vectors are constructed analogous to the Bravais lattice, where

$$\vec{G} = m_1 \vec{b}_1 + m_2 \vec{b}_2 + m_3 \vec{b}_3 \tag{2.22}$$

The volume of the unit cell in reciprocal space, called the Brillouin Zone, is



Figure 2.2: Brillouin Zones of common crystal structures. [14]

$$\vec{b}_1(\vec{b}_2 \times \vec{b}_3) = s \frac{(2\pi)^3}{\vec{a}_1(\vec{a}_2 \times \vec{a}_3)} = \frac{(2\pi)^3}{\Omega}$$
(2.23)

2.3 Energy Bands and Density of States

Figure 2.2 shows the Brillouin zone for common crystal structures. The notation used to indicate points in reciprocal space that have high symmetry was introduced by Bouckaert, Smolukowski, and Wigner [15]. The band structure calculations determine symmetry and angular momentum character of the energy states along the different directions in the Brillouin zone. When plotting the energy bands, the results of APW calculations are interpolated using a k-point mesh within the Brillouin zone. The band structure then shows the energy states along a particular path of Brillouin zone, as shown in Figure 2.3a. For a simple cubic structure, the path is typically $\Gamma - X - M - \Gamma - R - X|M - R$, as shown in Figure 2.2a. The same band structure calculations allow us to determine the DOS, which is the number of states per unit energy. The preferred method for calculating the DOS is the tetrahedron method [16], in which the eigenvalues, $\epsilon(k)$, are linearly interpolated between four k-points placed on the vertices of the tetrahedron according to the relationship

$$\epsilon(k) = \epsilon_0 + \vec{b}(\vec{k} - \vec{k}_0) \tag{2.24}$$

where ϵ_0 and \vec{b} are determined by the energies at the corners of the tetrahedron. Observing the band structure alongside the DOS, as in Figure 2.3b, we see that DOS is effectively a histogram of energy states.



Figure 2.3: Electronic Band Structure and DOS of ScTi.

2.4 The CsCl Structure

In this work, we construct diatomic compounds from the transition metals series in the Cesium Chloride (CsCl) structure, shown in Figure 2.4. The CsCl structure is in the $Pm\bar{3}m$ space group, which means it is of the simple cubic category. The use of the CsCl structure is motivated by our use of the Muffin-Tin approximation. Because the MTA creates a sphere



(a) CsCl Primitive Cell; Cs+ (Purple), Cl-(Green) [17]

(b) CsCl Simple Cubic structure Cs+ (Grey), Cl- (Green) [18]

Figure 2.4: Cesium Chloride structure

about each atom, such that each sphere touches its neighbor, we can consider the packing fraction of these spheres within the unit cell. The packing fraction is defined by

$$PF = \frac{[\# \text{ of atoms / unit cell}][\text{volume of a sphere}]}{[\text{volume of unit cell}]} = \frac{(2)(4/3\pi R^3)}{a^3}$$
(2.25)

In this work, the Muffin-Tin radius of the two elements are held equal for all calculations, such that each sphere touches its neighbor, but does not overlap. Then $R = \sqrt{3}a/4$ and the packing fraction is

$$PF_{CsCl} = 2(V_{sphere}) = (2)\left(\frac{4}{3}\pi\right)\left(\frac{\sqrt{3}a}{4}\right)^3 = 0.68$$
(2.26)

The only structure with a packing fraction greater than CsCl is an FCC structure. The high packing fraction of the CsCl structure makes it a suitable structure for the MTA.

2.5 Predicting Ferromagnetism

We have shown how DFT, coupled with the MT-APW method, allows us to solve Schrödingers equation for many-electron systems to calculate the ground state energy. Equation 2.17 also allows to directly calculate the available energy states to create the electronic band structure for the material and structure of interest. The electronic band structure, in turn, provides us with the density of states (DOS), which is the number of states per unit energy. Additionally, we can find the Fermi energy level, E_F , which is the maximum energy level that an electron can occupy at zero Kelvin. We can use these calculated properties, along with a few others, as parameters to predict the existence of ferromagnetic or superconducting properties.

The Stoner criterion is an inequality proposed by Stoner [4] to predict the occurrence of ferromagnetism, states as

$$N(E_F)I_S > 1 \tag{2.27}$$

where $N(E_F)$ is the DOS at the Fermi energy level, and I_S , as shown by Vosko and Perdew [19], is defined as

$$I_S = \int \gamma(r)^2 |K(r)| dr \qquad (2.28)$$

where γ is defined as

$$\gamma = \frac{1}{N(E_F)} \sum_{\ell} N_{\ell}(E_F) u_{\ell}^2(E_F)$$
(2.29)

where K(r) is an exchange and correlation enhancement of the external field due to magnetization, $u_{\ell}(E_F)$ is the radial wavfunction evaluated at the Fermi energy level, and $N_{\ell}(E_F)$ is the angular momentum decomposed DOS.

2.6 Predicting Superconductivity

To identify materials that possess the superconducting property, we use the work developed by McMillan [5] and Gaspari-Gyorffy [20]. Using BCS theory, McMillan developed an approach to determine the electron-phonon coupling constant, λ , defined as

$$\lambda_i = \frac{N(E_F)\langle I_i^2 \rangle}{M_i \langle \omega_i^2 \rangle} = \frac{\eta_i}{M_i \langle \omega_i^2 \rangle}$$
(2.30)

where M is the atomic mass, $\langle \omega^2 \rangle$ is the renormalized phonon frequency, and η is the Hopfield parameter [21]. The Hopfield parameter is the product of the DOS at the Fermi energy level, $N(E_F)$, with the square of the electron-ion coupling matrix element at E_F , averaged over the Brillouin zone, defined as

$$\langle I_i^2 \rangle = \frac{E_F}{\pi^2 N(E_F)^2} \sum_{\ell=0}^2 \frac{2(\ell+1)\sin^2(\delta_{\ell+1} - \delta_{\ell})N_{\ell+1}N_{\ell}}{N_{\ell+1}^{(1)}N_{\ell}^{(1)}}$$
(2.31)

where δ_{ℓ} are scattering phase shifts at E_F and N_{ℓ} is the angular momentum components at E_F . The $N_{\ell}^{(1)}$ parameter is the free-scatterer DOS, known as the rigid muffin-tin approximation by Gaspari and Gyorffy, defined as

$$N_{\ell}^{(1)} = \frac{\sqrt{E_F}}{\pi} (2\ell + 1) \int_0^{R_s} r^2 u_{\ell}^2(r, E_F) dr$$
(2.32)

where R_s is the radius of the muffin-tin sphere. The theory developed by McMillan to solve for the electron-phonon coupling constant, λ , also provided a way to calculate the transition temperature for superconductivity, T_C . McMillan proposed the following equation:

$$T_C = \frac{\langle \omega \rangle}{1.2} \exp\left(\frac{-1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right)$$
(2.33)

where the average phonon frequency, $\langle \omega \rangle$, is estimated from the Debye temperature, Θ_D , by the relationship

$$\langle \omega_i \rangle = \frac{\Theta_{D,i}}{\sqrt{2}} \tag{2.34}$$

The μ^* term is an estimation of the Coulomb pseudo-potential and typically has a value between 0.1 and 0.2. This estimated value will significantly affect the calculated value of T_C , and so it is meaningful to report μ^* alongside T_C . For a compound, each element contributes its own $\langle \omega \rangle$, from which we take the geometric average of the contributions to provide a singular value.

2.7 APW Codes and Usage

In this work, calculations were performed using an APW package developed at the Naval Research Laboratory (NRL) by Papaconstantopoulos, Klein, and Boyer, that implements the APW method within the local density approximation. The package also solves for the electron-phonon and ferromagnetic criterion. An automation of this package was done in 1996 by Brahim Akdim [22], a student of Dr. Papaconstantopoulos. This version was updated periodically by Dr. Papaconstantopoulos and other students. This author added several automation scripts to address the multiple calculations performed for this work. using the APW package. We performed calculations on over 435 diatomic compounds from the transition metal series, and all calculations are performed in the CsCl structure. However, for a given structure we must identify the ground state energy, which is dependent upon the separation distance between the atoms. Since we do not know what separation distance is the equilibrium lattice constant that yields the ground state energy, we must provide a series of guesses. For each lattice constant, we calculate the total energy, and then perform a fit of the total energies to find the minimum, or ground state energy, along with the equilibrium lattice constant. To perform the fit, we use the Birch-fit [23] formula, defined as

$$E(V) = \sum_{i}^{N} \alpha_{i} V^{2i/3}$$
 (2.35)

where V is the volume of the structure, α are the polynomial expansion coefficients, and N is the order of the fit. Typically, a third order fit sufficient for most systems, which expands to

$$E = E_0 + \frac{9}{8} B_0 V_0 \left[\left(\frac{V_0^{2/3}}{V} - 1 \right) \right]^2 + \frac{9}{16} B_0 V_0 (B_0' - 4) \left[\left(\frac{V_0^{4/3}}{V} - 1 \right) \right]^3$$
(2.36)

where E_0 is the equilibrium energy, V_0 is the equilibrium volume, B_0 is the equilibrium bulk modulus, and B'_0 is the pressure derivative of the bulk modulus. The bulk modulus is found by the second derivative of the energy with respect to volume, defined as

$$B = -V \frac{d^2 E}{dV^2} \tag{2.37}$$

Along with a starting lattice parameter, we must also provide a description of the elements within the compound of interest. For each element, this includes the atomic number, Z, and the number of valence electrons. The results of each calculation are stored in a database for archival and post-analysis, including band structure and DOS. The process for our calculations is captured in Figure 2.5.

Given the large number of compounds to explore in this work, it was prudent to automate the process of execution and archiving. We developed a small set of scripts capable of generating the requisite input file and collocating the relevant results for archival. The script reads a file containing the periodic table of elements and generates the input file with the appropriate atomic labels, weights, and determines the number of valence electrons. However, the challenge presented by automation exists not in the execution, but in the error handling. For a given calculation, we must provide an initial guess of the lattice constant, then perform the calculation for consecutive decrements of the initial lattice constant. It



Figure 2.5: Overview of APW calculation process.

is possible that the initial guess is inappropriate. The APW method may fail to find a minimum from the set of lattice constants. If this happens, we simply choose a smaller or larger initial lattice constant and re-run the calculation. The APW method may also fail to converge on a minimum energy for a given lattice constant, in which case the calculation will fail with no result. If this happens, we mark such failures in a separate file for further investigation. In general, compounds containing Cd or Hg tended to present challenges for automation. After calculations were completed for a set of compounds, a separate script was created to iterate over the set of results and check for completeness in terms of the parameters of interest and associated plots, and then collocate all relevant parameters, files, and figures to a staging directory for archival to the ESD.

Chapter 3: The Electronic Structures Database

The Electronic Structures Database (ESD) is an archive of results consisting of unary, binary, and some ternary compounds that is publicly available for search and reference. The monoatomic results are a complement to the work in [24] by providing the set of input parameters used in the calculations, along with detailed output files. The available diatomic compounds in the CsCl structure are the outcome of this work, and primarily consist of compounds from the transition metal series. Along with primary results such as equilibrium lattice constant, band structure, and DOS, the database provides a set of secondary result files that allow the work to be recreated. We will expand upon the purpose and meaning of the different results available from the archive.

The entry point to the ESD provides the user with set of options, shown in Figure 3.1. Users select the structure, compound, and property of interest from the menus. Upon submitting the request, the database will either return the associated result, or notify the user that the compound is not available. The following properties/results are available to the user:

- Energy Bands Returns figure of the associated band structure.
- Total Energy Returns figure of Birch Fit of Energy vs Lattice Constant and Energy vs Volume. The minimum Energy is then the equilibrium lattice constant.
- Density of States Returns figure of the associated DOS.
- Potential Energies Returns a file listing the potential energy, V(r), as a function of the distance, r, from the center of the atom.
- Charge Densities Returns a file listing the charge densities as a function of r. We note that the quantity listed $4\pi r^2 \rho(r)^2$.

Select the structure you want to view. *More structures are being generated.* **The following require 1 symbol.**

```
\bigcirc FCC \bigcirc BCC \bigcirc HCP \bigcirc DIA
The following require 2 symbols.
\bigcirc CU3AU \bigcirc FLO \bigcirc NACL \bigcirc CSCL
The following require 3 symbols.
O PEROV
Enter the symbol(s) of your choice from this chart:
                                                                 He
н
Li
   Be
                                                  С
                                                         0
                                                              F
                                                                 Ne
                                              R
                                                      Ν
Na
   Mg
                                              Αl
                                                  Si
                                                      Ρ
                                                          s
                                                             сl
                                                                 Ar
ĸ
    Ca
                                  Ni
                                      Cu
                                          Zn
                                              Ga
                                                  Ge
                                                      As
                                                        Se
                                                             Br
                                                                 Kr
       Sc Ti
               v
                   Cr
                       Mn
                           Fe
                              Со
              Nb Mo
                              Rh
Rb
   Sr
           Zr
                          Ru
                                  Pd
                                      Ag
                                          Cd
                                              In
                                                  Sn
                                                      Sb
                                                                 Xe
       Y
                      Tc
                                                         Te
                                                             Τ
   Ba La Hf
                          0s
                              Ir Pt
                                          Hg
                                              Τl
                                                 Pb
                                                     Bi
Cs
               Та
                  W
                       Re
                                     Au
                                                         Ро
                                                             At Rn
Symbol #1:
Symbol #2 [if needed]:
Symbol #3 [if needed]:
Select what type of information you would like to see.
 Energy Bands
  Submit
             Reset Form
```

Figure 3.1: Entry point to the ESD. Users select structure, compound, and property of interest from the menus. [25]

- Eigenvalues Returns a file of the calculated eigenvalues at the symmetry points in the Brillouin zone.
- Birch Fit Returns a file of the Birch Fit parameters.
- Other Results Returns a file that summarizes all results, along with additional calculated values. Additional values include the Bulk modulus and its derivative, the Hopfield parameter, η , and the Stoner parameter, I_S , as well as the Stoner criterion.

3.1 ESD Figures

The ESD provides access to the resulting figures for calculated equilibrium lattice constant, band structure, and DOS. The equilibrium lattice constant is found by performing a Birch Fit against the energy versus lattice constant, and the minimum energy denotes the equilibrium lattice constant, as shown in Figure 3.2b. The band structure is created from an interpolation of the calculated eigenvalues at the symmetry points in the Brillouin zone, as shown in Figure 3.2a. The solid horizontal line is the energy of the Fermi level. If the Fermi level intersects with the energy states, then the material is deemed a metal. Otherwise, the Fermi level will occur at a gap between bands, indicating that the material is either an insulator or a semi-conductor. We can also view the band structure from the perspective of the DOS, as shown in Figure 3.2c. The ESD provides the total DOS, along with the contributions from each orbital (i.e. s, p, d), and each component element of the compound.

The equilibrium lattice constant and DOS figures have an associated data file consisting of the values used to create the figure. The data file for E vs a is shown in Figure 3.3. The first column is the lattice constant and the second column is the calculated total energy. At the bottom, the equilibrium lattice constant, a_0 , and bulk modulus, K, as found by the Birch Fit, are shown. For the DOS figures, there are two files. The first file, shown in Figure 3.4a, is the data file used to create the figure, while the second file, shown in Figure 3.4b, provides the calculated value of the Fermi energy, E_F , along with the total DOS at the Fermi level, $N(E_F)$, and the contributions to the total from each orbital. The first data file has the following column format:

1. Index

- 2. Energy step
- 3. Number of electrons
- 4. Total DOS



Figure 3.2: Primary ESD Figures. [25] Sample figures shown are the result calculations performed for ScTi.

5-9. s-, p-, e_{g} -, t_{2g} , f-orbital contributions of the first component.

10-14. s-, p-, e_{g} -, t_{2g} , f-orbital contributions of the second component.

The second file provides the calculated Fermi energy, E_F . It has the following format:

- 1. Fermi energy, ${\cal E}_F$
- 2. Total DOS at the Fermi level, $N(E_F)$
- 3. Contributions to total DOS from s, p, e_g, t_{2g}, f -orbitals

7.000000	-3228.880743								
6.800000	-3228.907192								
6.600000	-3228.925718								
6.400000	-3228.934863								
6.200000	-3228.932435								
6.000000	-3228.916405								
6.337690	-3228.935822								
a = 6.33769 Bohrs Ko = 0.78196 Mbar									

Figure 3.3: E vs a data file. The first column is the lattice constant. The second column is the calculated energy. At the bottom are the equilibrium lattice constant and bulk modulus as found by the Birch Fit. Sample file is result of calculations performed for ScTi.

1 2 3 4 5	0.0000 0.0020 0.0040 0.0060 0.0080	0.0011 0.0016 0.0021 0.0028 0.0037	L 0.2056 5 0.2433 L 0.3079 8 0.3994 7 0.5179	0.0054 0.0057 0.0060 0.0063 0.0066 (a)	0.0004 0.0006 0.0009 0.0013 0.0018 DOS d	0.0008 0.0013 0.0021 0.0035 0.0057	0.0003 0.0005 0.0010 0.0017 0.0027 e to reci	0.0000 0.0000 0.0000 0.0000 0.0001	0.0018 0.0020 0.0023 0.0027 0.0031	0.0018 0.0020 0.0023 0.0027 0.0032	0.0002 0.0005 0.0011 0.0024 0.0043	0.0007 0.0009 0.0012 0.0017 0.0023	0.0000 0.0000 0.0000 0.0000 0.0001
	Sc Ti 0.55939 46.47786 0.55939 46.47786				0.30 0.41	186 2 473 2	. 19146 . 64283	APW 1.9300 5.2479	-DOS - 6 9. 2 15.	- 02976 53777	0.18700 0.13859		

(b) Calculated value of E_F , along with $N(E_F)$ and associated contributions.

Figure 3.4: Data files associated with DOS figures. Sample file is the result of calculations performed for ScTi.

3.2 Other ESD Data Files

The remaining options available to the user provide additional data files with calculated values. The Potential Energy data file provides the calculate potentials inside the Muffin-Tin sphere for monotonically increasing radii, along with the value of the constant potential used for the interstitial regions. The format of the Potential Energy data file, shown in Figure 3.5a, is as follows:

 Line 1: # of Values, Starting Point of Radial Mesh, Constant Potential in Interstitial Region, Muffin-Tin Radius, Element Label, Wigner-Seitz Radius

- Line 2: Increments at which Linear Radial Mesh step size is doubled
- Line 3 to N: Muffin-Tin radius, R, and Potential, V(R)

The Charge Densities data file provides the calculated charge densities for each Muffin-Tin sphere. The format of the Charge Density data file, shown in Figure 3.5b, is as follows:

- Column 1: Radius of the Muffin-Tin sphere, R
- Column 2: Total Charge Density, $4\pi R^2 \rho(R)$
- Column 3: Core Charge Density, which is the total charge density minus the charge density of the valence electrons

The Eigenvalues data file provides the calculated eigen-energies used to create the band structure plots shown earlier. The format of the Eigenvalues data file, shown in Figure 3.5c, is as follows:

- Column 1: Energy at the k-point, E(k)
- Column 2-6: Angular momentum character of the state for each s,p,e_g,t_{2g},f -orbital, $Q(\ell)$
- Column 7: The label for the symmetry point in the Brillouin zone
- Column 8: The label for the k-point vector
- Column 9: The label for the associated element(s) of interest

The Birch Fit data file, shown in Figure 3.5d, provides the Birch coefficients used to fit E vs a and E vs V figures shown earlier. The first line shows the order of the fit. The second line is the labels for each coefficient. The third line are the coefficients used in the fit. The remaining lines are the values calculated by finding the minimum energy of the fit.

The final option available to the user is summary file of the results associated with the compound, shown in Figure 3.6. This summary file includes the equilibrium lattice constant,

the minimum energy, the bulk modulus and its derivative. Additionally, the Fermi energy level, E_F , the DOS at the Fermi energy level, $N(E_F)$, the Hopfield parameter, η , and the Stoner parameter, I_S , are shown here.

The ESD provides an archive of results that allow users to access compounds of interest and provides them with the necessary information to recreate the results. The ESD can be found at http://esd.spacs.gmu.edu/db/.
533 0.000020010 0.070212 2.744300 1Sc 1 3.120504 32 64 96 128 160 192 224 256 288 0.200000000000D-04 0.2099865008455D+07 0.400000000000D-04 0.1049864788368D+07 0.600000000000D-04 0.6998646557843D+06 0.800000000000D-04 0.5248645589337D+06 0.100000000000D-03 0.4198644816364D+06 (a) Potential Energy data file 0.20000000000D-04 0.3737848840594D-04 0.37355315413250-04 0.40000000000D-04 0.1469636079932D-03 0.1468725815168D-03 0.600000000000D-04 0.3272414377871D-03 0.3270389353168D-03 0.800000000000D-04 0.5773373980329D-03 0.5769803034394D-03 0.10000000000D-03 0.8965936684521D-03 0.8960392494104D-03 1200000000000 03 0 12044660113200 02 0 12036726570550 02 (b) Charge density data file Q(p) E(k) Q(eg) Q(t2g) 0(s)0(f)k 0.16292 0.28227 0.00000 0.00000 0.00000 0.00000 GAM1 000 Sc 1 0.16292 0.32605 0.00000 0.00000 0.00000 0.00000 GAM1 000 Ti 1 0.43019 0.00000 0.00000 0.29594 0.00000 0.00000 GAM12 000 Sc 1 GAM12 0.43019 0.00000 0.00000 0.45240 0.00000 0.00000 000 Ti 1 0.43019 0.00000 0.00000 0.29594 0.00000 0.00000 GAM12 000 Sc 1 0.43019 0.00000 0.00000 0.45240 0.00000 0.00000 GAM12 000 Ti 1 0.66979 0.00000 0.00000 0.00000 0.24994 0.00000 GAM25P 000 Sc 1 0.66979 0.00000 0.00000 0.00000 0.70118 0.00000 GAM25P 000 Ti 1 0.66979 0.00000 0.00000 0.00000 0.24994 0.00000 GAM25P 000 Sc 1 0.66979 0.00000 0.00000 0.00000 0.70118 0.00000 GAM25P 000 Ti 1 0.66979 0.00000 0.00000 0.00000 0.24994 0.00000 GAM25P 000 Sc 1 0.66979 0.00000 0.00000 0.00000 0.70118 0.00000 GAM25P 000 Ti 1 0.80268 0.00000 0.00000 0.50308 0.00000 0.00000 GAM12 000 Sc 1 (c) Eigenvalues data file Order= 3 A1 A3 A4 A2 -6.526998141298E+00 -2.290673763297E+02 6.744806378538E+03 -5.742197075650E+04 Equilibrium parameters for the Birch-Murnaghan equation of order 3: Vo = 254.56207 Bohr**3 a = 6.33769 Bohrs Eo = -8.93542 Rydbergs Ko = 0.78196 Mbar Ko'= 2.83583 RMS error in energy fit = 0.00003 Rydbergs Maximum error in energy fit = -0.00005 Rydbergs

(d) Birch Fit data file

Figure 3.5: ESD Data files used for calculations. Sample files are the result of calculations performed for ScTi.

	••••••			
	•			
	 RESULTS OF THE A ScTi 	APW CALCULATION cscl		
			•	
IL/	ATTICE PARAMETERS IN BOHR	TOTAL ENERGY IN RYD	OBERG	
	7.00000	-3228.88074		
	6.60000	-3228.92572		
1	6.40000	-3228.93486		
	6.0000	- 3228.93244		
1	6.33769	- 3228.93582	2	
	••••••			
	* EQUITI TRRTIIN			
	* ScTi	cscl		
	•			
Ĩ.	ATTICE PARAMETERS IN BOHR	TOTAL ENERGY IN RYD	DBERG	
	6 22260			
	0.33/09	- 3228.9358/	2	
			·····.	
· ·	Volume Vo =	254.56207 (Bohr^3	3)	
i	Lattice constant ao =	6.33769 (Bohr)	
ļ 1	Bulk modulus Ko =	0.78196 (MBar)	
	Ko'=	2.83583		
1	RMS error in energy fit =	0.00003 (Ry)	
	•••••			
	•			
	 DENSITY OF STATES / ScTi 	AT THE FERMI ENERGY		
		cocc .		
	**********************	••••••	•	
Fermil	Energy Total DOS (Ry)(States/Ry) s	Decomposed DOS insi p eq	ide the muffi g t2g	in tins f
0.55939	46.47786 0.	30186 2.19146	1.93006 9.0	2976 0.18700
0.00939	40.4//80 0.	.414/3 2.04283 :	0.24/92 15.3	0.13859
Fermi-vetoc.	LLY (CM/S): 2.13041 X10E0			
Plasmon Ene	rgy (eV) : 33.07938			
Electron-io	n interaction (Hopfield pa	arameter (eV/A^2)): Sc 1.32321 Ti 1.63448		
		T 10.0555		
A	TOM 2 MUFFIN-TIN CHARG	E = 19.9003		
A	TOM 1 STONER I = 0	0.0028140		
A	TOM 2 STONER I = 0	0.0074780		
5	TONER CRITERION N*I = 6	0.4813		
NUMBER OF	ATOMS 2			

Figure 3.6: ESD Results Summary data file

Chapter 4: Results and Discussion

We apply the APW method with LDA functional for exchange and correlation to perform calculations to predict ferromagnetic or superconducting properties in diatomic compounds from the transition metal series. A total of 435 compounds were evaluated in this work. We compare the calculated equilibrium constant against the alternative Generalized Gradient Approximation (GGA) functional, and experimental results for 60 compounds that are known to exist (i.e. compounds that were synthesized), shown in Figure 4.1. We find that the APW method with LDA functional is in good agreement with the GGA functional and experiment. However, we note that the LDA functional has a tendency to underestimate the measured lattice constant, while the GGA functional has a tendency to overestimate the lattice constant. Additionally, the work of Reference [26] performed similar first-principles calculations to identify the ground state structure for 80 binary compounds, many of which are of the transition metal series. Their work confirms that CsCl is the ground state structure for AgMg, AgY, AuY, RhY, RuZr, RuTi, and TcTi, in agreement with our results. The ground state structure for compounds AgCd and AuSc were found to be degenerate and include the CsCl structure. The ground state structure for compounds AuCd and NbRu were found to be of the CsCl ground state, but only at high temperature. Additionally, their work predicts the CsCl ground state structure for CdY, MoNb, NbTc, and TcZr. The present work contains additional calculations beyond that of Reference [26], in that we focus on the subset of compounds that meet the criteria for possessing either ferromagnetic or superconducting properties. We use the Stoner criterion to identify compounds that possess the ferromagnetic property. We also calculate the average phonon frequency, $\langle \omega \rangle$, the electron-phonon coupling constant, λ , and the superconducting critical temperature, T_C , to identify compounds that possess the superconducting property.



Figure 4.1: Comparison of calculated equilibrium lattice constant from APW method with LDA functional, against alternative GGA functional and Experiment for compounds known to occur naturally. [27]

4.1 Ferromagnets

We identified 63 compounds that met the Stoner criterion, as shown in Table 4.1, thereby possessing the ferromagnetic property. Many of these compounds contain Iron (Fe), Cobalt (Co), Nickel (Ni), or Manganese (Mn), which are known to be inherently ferromagnetic elements. However, some compounds have a calculated Stoner parameter very close to the Stoner criterion, but are excluded from our results. For example, in [28] the authors explore the magnetization and magnetic structure of MnZn in the CsCl structure, and they note that this material exhibits strong ferromagnetism at room temperature. Our calculations found MnZn to have a Stoner criterion of $N(E_F)I_S \approx 0.99$, which does not exactly meet the Stoner criterion. But the compound Iron-Cadmium (FeCd) is of particular interest because it displays an exceedingly large Stoner criterion greater than 5. We will explore the FeCd compound further in the following section, and compare it against the VRh compound, whose Stoner criterion is found to be close to one.

Table 4.1: Compounds predicted to possess Ferromagnetic properties shown alongside their respective Stoner criterion. We *emphasize* those compounds that are known to occur naturally in the CsCl structure. Compunds in **bold** are found to have very large values of the Stoner criterion. Compounds found to possess ferromagnetic properties are eliminated from the set of identified superconductors.

ScCr	1.126	ScMn	1.329	VFe	1.053	VCo	1.049	VZr	1.001
VRh	1.001	VAu	1.176	CrFe	1.820	CrNi	1.148	CrY	1.708
CrRu	1.090	CrPd	1.388	CrAg	1.301	CrCd	1.069	CrLu	1.379
CrIr	1.114	CrPt	1.371	CrAu	1.365	MnFe	1.383	MnCo	1.227
MnNi	1.021	MnY	2.028	MnRu	1.020	MnRh	1.097	MnPd	1.393
MnAg	1.013	MnCd	1.059	MnLu	1.639	MnIr	1.145	MnPt	1.445
FeCo	1.982	FeCu	1.153	FeZn	2.308	FeY	1.548	FeNb	1.112
FeMo	1.444	FeTc	1.746	FeRu	2.575	FeRh	1.870	FeAg	1.264
FeCd	5.442	FeTa	1.062	FeRe	1.066	FeOs	1.594	FeIr	2.098
FeHg	3.066	CoNi	2.839	CoCu	2.535	CoZn	1.206	CoRu	1.360
CoPd	1.803	CoAg	3.240	CoCd	1.448	CoOs	1.034	CoPt	1.173
CoAu	1.756	CoHg	1.124	CuRh	1.045	RuCd	2.718	RuIr	1.112
RhPd	1.007	RhAg	1.170	RhAu	1.060				

4.2 Ferromagnets FeCd and VRh

A key indicator of ferromagnetic behavior is a high DOS at the Fermi level, $N(E_F)$, and a strong Coulombic interaction. In Table 4.2, we show the calculated parameters for FeCd and VRh. We note that the equilibrium lattice constant is small for both (i.e. < 6 a.u.) which contributes to a strong Coulombic interaction. Additionally, we note that the DOS at the Fermi level, $N(E_F)$, is large for both. Since the Stoner criterion is found by the product $N(E_F)I_S$, then a large $N(E_F)$ yields a large Stoner criterion. We present the decomposed DOS for both FeCd and VRh compounds in Figure 4.2. From the decomposed DOS in Figures 4.2a and 4.2b, we note that the DOS is dominated by contributions from the *d*-orbitals. In particular, *d*-orbital contributions by Fe and V are the most dominant.

We expect the energy contributions to be highest from *d*-orbital electrons because their orbit is further away from the nucleus which decreases the electron-nucleus potential. The energy levels of *d*-orbital electrons are degenerate, and are split into two: e_g and t_{2g} . Electrons with lower energy occupy the t_{2g} level, and those with higher energy occupy the



Figure 4.2: DOS of FeCd and VRh.

 e_g level. In Table 4.3, we show the contributions to $N(E_F)$ from each orbital. For FeCd, the t_{2g} energy level in Fe contributes the most. For VRh, the t_{2g} level in V contributes the most, also. Since the DOS is directly related to the electron density, then for FeCd we can say that the large difference between the e_g and t_{2g} DOS contributions means a higher density of unpaired electrons that contribute to its ferromagnetic behavior. Similarly, VRh has a smaller difference between the e_g and t_{2g} energy levels, meaning a lower density of unpaired electrons that contribute to its ferromagnetic behavior, and thus a lower Stoner criterion.

If we compare FeCd and VRh to HfOs, whose Stoner criterion was calculated to be the smallest in our data set, then we can observe the distinction in contributions to $N(E_F)$. For HfOs, the equilibrium lattice constant is larger than that of FeCd and VRh, meaning a

	a_0 (a.u)	E_F (Ry)	$N(E_F)$ (states/Ry)	I_S (Ry)	$N(E_F)I_S$
FeCd	5.7	0.64	189.4		5.44
Fe				0.0287	
Cd				0.00003	
VRh	5.6	0.77	68.95		1.001
V				0.0121	
Rh				0.0025	
HfOs	6.1	0.77	4.45		0.03
Hf				0.0037	
Os				0.0031	

Table 4.2: Comparison of $N(E_F)$ between FeCd, VRh, and HfOs. We note that smaller equilibrium lattice constant increase Coulombic interaction and large $N(E_F)$ are indicative of ferromagnetic properties.

Table 4.3: Comparison of s-, p-, and d-orbital contributions to $N(E_F)$. We note the important role that d-orbitals play in ferromagnetic behavior.

	s	p	e_g	t_{2g}	f
Fe	0.36656	0.58732	21.91542	155.886	0.07305
Cd	0.16091	0.47240	0.03663	4.65750	0.92138
V	0.29709	0.54263	15.86187	25.97968	0.14682
Rh	0.66265	1.47185	15.92078	3.51582	0.43442
Hf	0.02345	0.33514	1.03103	0.13535	0.04609
Os	0.05048	0.50460	0.61432	0.40844	0.08269

weaker Coulombic interaction. Only the e_g -orbitals are the primary contributors to $N(E_F)$, which means a large portion of the electron density exists close to the nucleus, minimizing their interaction with neighboring atoms. Additionally, the e_g and t_{2g} energy levels of Os are nearly equal, meaning only a small density of unpaired electrons exists to contribute to any form of magnetic behavior, and thus a small Stoner criterion. Here we see the large role that the *d*-orbital electrons perform, and in particular the need for a significant difference in electron density between the e_g and t_{2g} energy levels.

As further verification of our results, [29] compares the characterization of magnetism in FeRe samples with first principles calculations, demonstrating that our prediction of ferromagnetic FeRe is reasonable. Additionally, [30] characterized the magnetic properties of MnRh in a CsCl structure, again demonstrating that our prediction of ferromagnetic MnRh is reasonable. In [30], the authors also compare their work to experimental results of FeRh, another compound that we predicted to possess ferromagnetic properties.

4.3 Superconductors

In order to identify compounds that possess the superconducting property, we calculate the electron-phonon coupling constant, λ , the average phonon frequency, $\langle \omega \rangle$, and the critical temperature, T_C . By definition of BCS theory, a superconductor cannot also be ferromagnetic because a superconductor has no observable magnetic field. Compounds found to possess the ferromagnetic property are then removed from the subset of identified superconductors. However, the model used to calculate T_C is heavily influenced by λ and μ^* . If λ is sufficiently small, then T_C can tend towards infinity, which is physically impossible. Compounds that experience an exceedingly large T_C are eliminated from the set. Conversely, certain combinations of η , λ , and $\langle \omega \rangle$ will yield a T_C so small, that it is effectively zero. While such results are theoretically meaningful, they are not useful for comparison in the context of this work. Compounds that experience a T_C of zero are eliminated from the set. The final set of compounds found to possess superconducting properties consists of 239 compounds from the transition metal series. If we sort the set by average phonon frequency, we find that compounds paired with Hg tend to have the lowest phonon frequency, and compounds paired with Nb tend to have the highest phonon frequency. In particular, VRu and TiRu are known superconductors [31] that we can compare our calculations against. We will explore these compounds, and others, in more detail in subsequent sections.

4.4 Superconductors in the CsCl Structure

This work uses the McMillan-Gaspari-Gyorffy theory, which is derived from BCS theory, to model electron interactions within a lattice to predict fundamental superconductor properties, such as the electron-phonon interaction and the critical temperature. BCS theory relates the interaction of electrons with lattice vibrations, known as electron-phonon interactions. In a conductor, an electric field causes free electrons to move within the lattice structure. As electrons flow within the lattice, they collide with their neighbors causing resistance to the flow of electrons. Moving electrons attract positive charges in the lattice. causing the lattice to slightly deform. This deformation, called a phonon, causes another electron with opposite spin to occupy the region of higher positive charge density. Now the movement of two electrons are correlated with each other, creating a Cooper pair. As more of these Cooper pairs form, fewer collisions occur, causing the resistance to go to zero. In the superconducting state, the magnetic field of the surface current will cancel the magnetic field within the bulk of the material, such that the measured magnetic flux is zero. This behavior is called the Meissner effect, and is predicted by BCS theory. It is for this reason that we eliminate the set of predicted ferromagnets from the set of predicted superconductors.

Furthermore, we use the work by McMillan-Gaspari-Gyorffy to calculate the electronphonon coupling constant, λ , the average phonon frequency, $\langle \omega \rangle$, and the critical temperature, T_C . The calculation of both T_C and λ is dependent upon $\langle \omega \rangle$, as described in Equation 2.33. By Equation 2.34, the average phonon frequency is approximately related to the Debye temperature. From Equations 2.30, 2.31, and 2.32, we note that the value of the electron-phonon coupling constant is the ratio of the Hopfield parameter, η , divided by the force constant, $M\langle \omega^2 \rangle$. T_C is dependent upon one more parameter; an estimation of the Coulomb pseudopotential, called μ^* . The Coulomb repulsion is called μ , and is defined as $N(E_F)V_C$, where V_C is the Coulomb potential. The Coulomb pseudopotential, μ^* , is estimated from our prediction of $N(E_F)$. However, the computation of μ^* is generally deemed to be computationally demanding, and can be treated instead as a free parameter

Table 4.4: Known superconductors in the CsCl structure, and their T_C . [31]

AgLu	0.33K	AgY	0.33K	AuLu	$< 0.35 \mathrm{K}$	CaHg	1.6K	TiOs	0.46K
CuY	0.33K	TiRu	$1.07 \mathrm{K}$	VRu	4.0K	ZnY	0.33K		

to fit the experimental value of T_C [32]. For the following results, we chose to fit against the experimental value of VRu, whose $T_C = 4.0$ K [31], and we chose to apply $\mu^* = 0.18$ for all calculations.

There is one more feature that impacts the results of our calculations, and that is the crystal structure. The constant feature of this work is the CsCl structure. However, within the scope of superconductors, the prevailing wisdom is that the CsCl structure is not favorable to achieving the superconductor state. Reasons for this are discussed in [33], in which the author postulates that the valence electron-to-atom ratios are too low, which tend to yield low transition temperatures. Additionally, they suggest that certain compounds in the CsCl structure possess particular instabilities that make them unsuitable as superconductors. According to [31], only a handful of compounds that exist in the CsCl structure are known superconductors, which we show in Table 4.4. These compounds have a low T_C of 1K or less, with the exception of VRu which has $T_C = 4.0K$.

Of the 435 compounds explored in this work, we eliminated compounds from the set of superconductors which we had previously predicted it to be ferromagnetic. Compounds whose calculated T_C were found to be outside reasonable boundaries have very low electronphonon coupling values. In Figure 4.3, we show the behavior of T_C with respect to a changing λ , while holding the average phonon frequency constant at $\langle \omega \rangle = 200$. We see that for $\lambda < 0.3$, the calculated T_C is negligible. For this reason, we eliminated those compounds from the set of superconductors. We identified 239 compounds to be possible superconductors. Given the aforementioned possible instabilities in the CsCl structure, we will focus our discussion on those compounds that are known to be at least thermodynamically stable in the CsCl structure, of which there are 25. These compounds, and their calculated T_C , are shown in Table 4.5.

ScAu	0.0006	ScHg	2.942	TiCo	0.498	TiNi	0.112
TiTc	0.333	TiRh	0.0281	TiPd	0.386	TiRe	0.0012
TiPt	0.102	TiAu	0.634	VMn	0.0001	VTc	0.0001
VRu	5.365	VOs	4.731	MnAu	0.183	MnHg	0.180
CoZr	0.0385	CuZr	0.0193	ZnY	2.616	YHg	0.958
ZrRh	0.0022	ZrPd	6.335	ZrIr	0.0002	NbRu	5.371
RuTa	2.339						

Table 4.5: Predicted superconductors that are known to be thermodynamically stable in the CsCl structure, and their T_C , in degrees Kelvin.

From Table 4.5, we see that the prevailing wisdom persists, wherein the calculated T_C is low for all compounds. We note that for VRu, we calculated $T_C \approx 5.3K$, and not 4.0K as experimentally measured. We can see that compounds paired with Vanadium have a high T_C . But the compound ZrPd is of particular interest, with a calculated T_C of 6.34K.

We stated earlier that T_C is dependent upon the electron-phonon coupling constant, λ , the average phonon frequency, $\langle \omega \rangle$, and the 'renormalized' Coulomb repulsion, μ^* . Our calculations are performed with a fixed $\mu^* = 0.18$. Then the contributing parameters to T_C are the calculated λ and $\langle \omega \rangle$. The average phonon frequency is determined by a given Debye temperature, Θ_D . The electron-phonon coupling constant is determined by the ratio of the Hopfield parameter, η , to the quantity $M \langle \omega^2 \rangle$. To calculate a high T_C , we require a sufficiently large electron-phonon coupling constant, λ , and a large average phonon frequency, $\langle \omega^2 \rangle$. And a large λ requires a large Hopfield parameter, η , but a small $M \langle \omega^2 \rangle$. But we also want a large $\langle \omega \rangle$, which is taken to be the geometric mean of the average phonon frequency from each component element. We see that a high T_C requires balancing the average phonon frequency to be large enough to motivate electron-phonon coupling, but not so large that it eliminates the contributions of the Hopfield parameter.

In Table 4.6, we highlight the outliers from our set of predicted superconductors. The compound ZrPd clearly possesses the highest T_C , while RuTa possesses the lowest T_C . ZrPd has a small equilibrium lattice constant, which yields a higher $N(E_F)$. The higher $N(E_F)$ motivates a larger η . Since both possess a high Debye temperature, the average phonon



Figure 4.3: $T_C \vee \lambda$. We eliminate compounds from the set of superconductors when $\lambda < 0.3$. $\langle \omega \rangle = 200.0$ in this figure.

frequency is proportionally large, as well. With the exception of Ta, none of the elements are particularly heavy, so the quantity $M\langle\omega^2\rangle$ is sufficiently small, so as not to eliminate the contributions from η . Hence, ZrPd possesses a sufficiently large electron-phonon coupling constant; thus, a high T_C . Conversely, RuTa has a much lower $N(E_F)$ which yields a much smaller η . The large Debye temperature effectively eliminates the contributions by η , yielding a small electron-phonon coupling constant; thus, a lower T_C . However, the AuHg compound presents some interesting contrasts to the others. The equilibrium lattice constant is comparatively larger than the others, and hence a much lower $N(E_F)$ and η . The Debye temperatures are much lower, and hence a much lower average phonon frequency. In fact, the AuHg compound possesses the lowest average phonon frequency of all the compounds in the set. But the low $\langle\omega\rangle$ is what allows the compound to retain the contributions by η , yielding a sufficiently high electron-phonon coupling constant. By investigating the outliers, we can see the how the contributions by η , $\langle\omega\rangle$, and λ must be balanced in order to yield a high T_C . Because the compound ZrPd is known to be stable in the CsCl structure, there is value in exploring its behavior experimentally.

	$ \begin{array}{c} a_0 \\ (a.u.) \end{array} $	$\frac{N(E_F)}{(\text{states/Ry})}$	λ	$\langle \omega \rangle$	η (eV/Å ²)	Θ_D (K)	$M\langle \omega^2 \rangle$	T_C (K)
Zr-Pd	6.23	63.27	0.8738	199.67				6.33
Zr					1.25	291.0	1.43	
Pd					4.91	274.0	5.62	
Au-Hg	6.29	9.36	0.4248	77.02				0.035
Au					0.92	165.0	2.17	
Hg					0.21	71.9	0.49	
Ru-Ta	5.91	46.7	0.62	268.33				2.34
Ru					9.16	600.0	14.8	
Ta					3.10	240.0	5.00	

Table 4.6: Contributing parameters to T_C for ZrPd, AuHg, and RuTa. For each compound, we present the contributions from each element.

4.5 Additional Superconductors

In the previous section we focused on compounds that are known to be thermodynamically stable in the CsCl structure. However, our calculations also identified a set of 14 compounds whose $T_c > 10K$, but are not known to exist in the CsCl. These compounds are shown in Table 4.7. The compounds TiNb and TiV are the obvious outliers, with T_c of 21.865K and 22.165K, respectively. From the previous discussion, we can understand how these compounds were calculated to possess such a high T_c . Both compounds effectively maximize all of the relevant parameters to create the conditions for a high T_c . Their small equilibrium lattice constants, a_0 , motivate electron interactions, which is also seen by their large electron-phonon coupling constant, λ . Both possess high Debye temperatures, Θ_D , which promotes their high phonon frequencies, $\langle \omega \rangle$. Moreover, the Hopfield parameter, η , is quite large not just in both compounds, but also for each component.

The compound TiNb is a well known superconductor [31] with many applications, and is

HfTa	10.034	ScMo	10.256	OsHg	12.364	CrMn	12.888
VNb	14.650	TiTa	14.830	ZrTa	15.581	NbHf	16.637
VHf	17.614	MnTc	18.257	MnRe	18.821	ZrNb	18.940
TiNb	21.865	TiV	22.165				

Table 4.7: Additional predicted superconductors and their T_C , in degrees Kelvin.

considered the workhorse of commercial superconductors because the critical temperature is $\approx 10K$. According to [34], TiNb and its alloys tend to have a composition of more Ti than Nb, while our ideal CsCl structure possesses equal amounts of both components. Moreover, Ti alloys, such as TiV and TiTa, are common in studies of superconducting materials [35], but not in the CsCl structure. Additionally, ZrNb was studied in [36] to determine its elastic constants in the BCC structure over the temperatures 4.2K to 300K. It is reasonable to conclude that the compounds shown in Table 4.7 can achieve a $T_c > 10K$, but not in the CsCl structure.

Table 4.8: Contributing parameters to T_C for TiNb and TiV. For each compound, we present the contributions from each element.

	$\begin{bmatrix} a_0 \\ (a.u.) \end{bmatrix}$	$N(E_F)$ (states/Ry)	λ	$\langle \omega \rangle$	η (eV/Å ²)	Θ_D (K)	$M\langle \omega^2 \rangle$	T_C (K)
Ti-Nb	6.04	57.34	1.55	240.34				21.865
Ti					4.50	420.0	2.90	
Nb					5.93	275.0	3.83	
Ti-V	5.74	59.84	1.38	282.49				22.165
Ti					4.26	420.0	3.09	
V					5.33	380.0	3.86	

Chapter 5: Summary and Future Work

In this work, we explored 435 binary compounds from the transition metal series in the CsCl structure in order to predict which compounds possess either ferromagnetic or superconducting properties. We applied the Stoner criterion to identify 63 compounds that possess the ferromagnetic property. In particular, we predict the compound FeCd to possess large Stoner criterion greater than 5. We used the work of McMillan and Gaspari-Gyorffy to identify the superconducting properties of 239 compounds. In particular, we predict the compound ZrPd to possess a superconducting critical temperature of $\approx 6.3K$. Additionally, we found TiNb and TiV to possess a high T_c of 21.9K and 22.2K, respectively. Moreover, TiNb is a well known superconductor used in many commercial applications, but it is not employed in the CsCl structure. We discussed those compounds whose properties represented the outliers of their respective sets. In ferromagnetic compounds, we noted that a small equilibrium lattice constant motivates a strong Coulombic interaction, which yields a large $N(E_F)$. Also, we noted the strong role that d-orbital electrons play in ferromagnetic compounds. In particular, a large difference in DOS between e_g and t_{2g} energy levels is indicative of ferromagnetic behavior. For those compounds found to possess valid superconducting properties, we noted the need to balance the contributions from the Hopfield parameter, η , the average phonon frequency, $\langle \omega \rangle$, and the electron-phonon coupling constant, λ , in order to achieve a high critical temperature, T_C . The results of our calculations are archived in our Electronic Structures Database (ESD), which is publicly available online [25]. The contents of our database include relevant figures and output files, such that users can recreate our work using comparable tools.

Despite the extended nature of our calculations, there exists many opportunities to expand upon it. A constant feature of our calculations is the CsCl structure. However, this structure may not be the ground state structure for many of the compounds we investigated. We identified 60 compounds that are known to be thermodynamically stable, and the work of [26] provides an in-depth analysis of 80 binary compounds to identify their ground state structure over a range of percent weight compositions. Knowledge of the ground state structure would improve the validity of our results. In addition to the ground state structure, it would be meaningful to calculate the elastic constants to determine the thermodynamic stability of each compound, beyond what is already documented. This would be particularly useful to the experimentalist interested in synthesizing any of these compounds. Exploring different crystal structures may also improve the validity of our predictions of superconductors. As noted by [33], the CsCl structure is sometimes not favorable for achieving the superconducting state.

It would also be useful to expand upon those compounds found to be ferromagnetic. In particular, performing a spin-polarized calculation would provide insight into the difference between spin "up" and spin "down" states, and allow us to predict the magnetic moment which can be used to calculate macroscopic material properties, such as the magnetic flux density and field strength. Such quantities could be useful to the experimentalist. It would also provide an additional form of comparison with similar first principles calculations. Additionally, it is possible to construct Tight-Binding Hamiltonian profiles of each compound by performing a fit against the first-principles APW data generated in this work.

The ESD also provides many opportunities for expansion. In its current state, users can choose from the set of compounds for which calculations have been performed, and review the results provided. However, the ESD does require a more advanced search capability that would allow users to access groups of compounds with similar properties of interest, instead of one at a time. Also, providing a real-time rendering of the band structure and DOS figures would improve the readability of the results. In addition, the ability to export the data files to more common file formats would improve the ability to compare results with other first principles calculations.

Appendix A: Appendix

Compound	a ₀ (a.u.)	$N(E_F)$ (states/Ry)	$\mathbf{N}(\mathbf{E_F})\mathbf{I_S}$	$\langle \omega \rangle$	λ	$\mathbf{T_C}(\mathbf{K})$
ScTi	6.338	68.782	0.729	274.955	0.686	3.860
Sc V	6.080	58.881	0.720	261.534	0.860	7.935
ScCr	5.920	75.972	1.126	336.749	0.697	5.041
ScMn	5.813	74.258	1.329	271.662	0.745	5.234
ScFe	5.751	44.560	0.768	290.861	0.421	0.119
ScCo	5.751	11.431	0.187	283.019	0.082	0.000
ScNi	5.852	14.754	0.155	284.605	0.185	0.000
ScCu	6.006	21.267	0.202	248.475	0.278	0.000
ScZn	6.173	0.000	0.293	242.611	0.299	0.000
ScGa	6.204	10.223	0.143	240.000	0.370	0.014
ScY	7.027	33.302	0.308	224.499	0.333	0.001
ScZr	6.608	45.031	0.414	228.867	0.651	2.563
ScNb	6.307	38.903	0.365	222.486	0.925	8.198
ScMo	6.129	58.704	0.619	284.605	0.917	10.256
ScTc	6.019	34.008	0.384	271.993	0.471	0.367
ScRu	5.955	24.213	0.249	328.634	0.273	0.000
ScRh	5.994	8.429	0.082	293.939	0.080	0.000
ScPd	6.141	15.281	0.141	222.081	0.234	0.000
ScAg	6.341	17.698	0.172	201.246	0.207	0.000
ScCd	6.531	26.594	0.317	193.959	0.208	0.000
ScLu	6.873	64.634	0.594	194.422	0.610	1.587
				Continu	ued on r	next page

Table A.1: Listing of calculated values for all compounds. Ferromagnets are highlighted in **bold**. Superconductors are highlighted in *italics*.

Compound	a ₀ (a.u.)	$\mathbf{N}(\mathbf{E_F})$ (states/Ry)	$\mathbf{N}(\mathbf{E_F})\mathbf{I_S}$	$\langle \omega \rangle$	λ	$\mathbf{T_C}(\mathbf{K})$
ScHf	6.580	57.955	0.527	212.979	0.687	3.017
Sc Ta	6.328	47.673	0.428	207.846	0.929	7.727
Sc W	6.161	49.205	0.467	268.328	0.728	4.760
ScRe	6.051	40.141	0.447	278.209	0.496	0.591
ScOs	6.008	32.944	0.352	300.000	0.335	0.002
ScIr	6.026	6.684	0.068	274.955	0.047	0.000
ScPt	6.150	14.048	0.120	207.846	0.243	0.000
ScAu	6.340	23.096	0.250	172.337	0.328	0.001
ScHg	6.476	34.793	0.472	113.763	0.814	2.942
TiV	5.743	60.024	0.634	282.489	1.384	22.165
TiCr	5.599	54.661	0.681	363.731	0.747	7.074
TiMn	5.503	20.333	0.288	293.428	0.400	0.060
TiFe	5.465	6.557	0.073	314.166	0.163	0.000
TiCo	5.495	36.331	0.506	305.696	0.480	0.498
TiNi	5.568	40.583	0.499	307.409	0.417	0.112
TiCu	5.685	67.550	0.934	268.384	0.578	1.625
TiZn	5.805	4.829	0.080	262.050	0.048	0.000
TiGa	5.866	44.330	0.728	259.230	0.538	1.001
TiY	6.645	57.620	0.699	242.487	0.521	0.752
TiZr	6.283	44.522	0.458	247.204	0.744	4.737
TiNb	6.039	57.477	0.533	240.312	1.551	21.865
TiMo	5.864	44.430	0.409	307.409	0.826	8.296
TiTc	5.769	21.416	0.193	293.786	0.462	0.333
TiRu	5.729	7.543	0.072	354.965	0.151	0.000
				Contin	ued on r	next page

Table A.1 – continued from previous page

Compound	a ₀ (a.u.)	$\mathbf{N}(\mathbf{E_F}) \text{ (states/Ry)}$	$\mathbf{N}(\mathbf{E_F})\mathbf{I_S}$	$\langle \omega \rangle$	λ	$\mathbf{T_C}(\mathbf{K})$
TiRh	5.780	36.923	0.415	317.490	0.379	0.028
TiPd	5.893	40.354	0.524	239.875	0.480	0.386
TiAg	6.047	67.261	0.977	217.371	0.534	0.807
TiCd	6.186	1.706	0.026	209.499	0.011	0.000
TiLu	6.506	58.720	0.683	210.000	0.576	1.254
TiHf	6.263	54.801	0.542	230.043	0.768	4.933
TiTa	6.042	54.400	0.495	224.499	1.235	14.830
TiW	5.896	46.254	0.409	289.828	0.806	7.262
TiRe	5.811	19.693	0.178	300.500	0.330	0.001
TiOs	5.781	5.416	0.048	324.037	0.121	0.000
TiIr	5.828	38.274	0.420	296.985	0.387	0.038
TiPt	5.931	32.304	0.397	224.499	0.425	0.102
TiAu	6.068	45.501	0.673	186.145	0.528	0.634
TiHg	6.212	18.020	0.334	122.878	0.387	0.015
VCr	5.384	25.716	0.317	345.977	0.484	0.599
VMn	5.317	8.517	0.102	279.106	0.306	0.000
VFe	5.307	67.162	1.053	298.831	0.997	13.141
VCo	5.326	73.798	1.049	290.775	0.977	12.192
VNi	5.378	51.180	0.728	292.404	0.609	2.374
VCu	5.468	14.497	0.221	255.284	0.274	0.000
VZn	5.584	28.512	0.604	249.259	0.346	0.003
VGa	5.645	39.968	0.760	246.577	0.603	1.891
VGe	5.676	29.824	0.508	266.571	0.558	1.309
VY	6.422	68.543	0.962	230.651	0.740	4.333
				Contin	ued on r	next page

Table A.1 – continued from previous page

Compound	a ₀ (a.u.)	$\mathbf{N}(\mathbf{E_F})$ (states/Ry)	$\mathbf{N}(\mathbf{E_F})\mathbf{I_S}$	$\langle \omega \rangle$	λ	$\mathbf{T_C}(\mathbf{K})$
VZr	6.104	81.360	1.001	235.138	1.523	20.924
VNb	5.857	43.424	0.483	228.583	1.212	14.650
VMo	5.697	16.345	0.150	292.404	0.444	0.224
VTc	5.627	9.336	0.095	279.446	0.302	0.000
VRu	5.595	38.857	0.613	337.639	0.707	5.365
VRh	5.641	69.387	1.001	301.993	0.780	6.827
VPd	5.729	60.125	0.974	228.167	0.741	4.313
VAg	5.856	21.621	0.332	206.761	0.252	0.000
VCd	5.980	36.408	0.726	199.274	0.279	0.000
VLu	6.251	59.155	0.804	199.750	0.786	4.623
VHf	6.057	74.888	0.872	218.815	1.409	17.614
VTa	5.868	38.936	0.433	213.542	0.994	9.312
VW	5.728	24.659	0.251	275.681	0.518	0.817
VRe	5.663	12.237	0.121	285.832	0.352	0.006
VOs	5.639	31.848	0.503	308.221	0.701	4.731
VIr	5.689	65.433	0.837	282.489	0.741	5.341
VPt	5.785	62.708	0.991	213.542	0.772	4.657
VAu	5.900	68.806	1.176	177.059	0.773	3.883
VHg	6.016	42.253	0.873	116.880	0.892	3.924
CrMn	5.217	42.097	0.642	359.374	0.915	12.888
CrFe	5.203	108.152	1.820	384.773	1.000	17.031
CrCo	5.215	59.600	0.938	374.400	0.530	1.309
CrNi	5.257	72.845	1.148	376.497	0.483	0.644
CrCu	5.335	45.069	0.834	328.702	0.372	0.021
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Table A.1 – continued from previous page

Compound	a ₀ (a.u.)	$\mathbf{N}(\mathbf{E_F})$ (states/Ry)	$\mathbf{N}(\mathbf{E_F})\mathbf{I_S}$	$\langle \omega \rangle$	λ	$\mathbf{T_C}(\mathbf{K})$		
CrZn	5.441	41.442	0.980	320.944	0.182	0.000		
CrY	6.299	101.794	1.708	296.985	0.572	1.698		
CrZr	5.969	62.072	0.867	302.762	0.715	5.022		
CrNb	5.739	17.811	0.231	294.321	0.317	0.000		
CrMo	5.611	16.426	0.217	376.497	0.216	0.000		
CrTc	5.531	36.595	0.541	359.812	0.611	2.953		
CrRu	5.509	64.335	1.090	434.741	0.464	0.514		
CrPd	5.623	76.246	1.388	293.786	0.625	2.704		
CrAg	5.741	66.173	1.301	266.224	0.427	0.129		
CrCd	5.856	44.854	1.069	256.583	0.143	0.000		
CrLu	6.116	85.634	1.379	257.196	0.614	2.169		
CrHf	5.939	57.568	0.866	281.745	0.523	0.905		
CrTa	5.735	31.793	0.458	274.955	0.367	0.014		
CrW	5.635	15.870	0.229	354.965	0.176	0.000		
CrRe	5.571	30.114	0.410	368.035	0.446	0.292		
CrOs	5.552	50.166	0.806	396.863	0.435	0.239		
CrIr	5.591	81.521	1.114	363.731	0.463	0.418		
CrPt	5.680	78.750	1.371	274.955	0.632	2.682		
CrAu	5.795	66.929	1.365	227.980	0.629	2.177		
CrHg	5.867	39.688	0.935	150.494	0.574	0.879		
MnFe	5.139	81.495	1.383	310.403	0.910	10.960		
MnCo	5.146	76.188	1.226	302.035	0.847	8.781		
MnNi	5.178	57.390	1.021	303.727	0.689	4.351		
MnCu	5.250	33.891	0.762	265.170	0.400	0.055		
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Table A.1 – continued from previous page

Compound	a ₀ (a.u.)	$\mathbf{N}(\mathbf{E_F})$ (states/Ry)	$\mathbf{N}(\mathbf{E_F})\mathbf{I_S}$	$\langle \omega \rangle$	λ	$\mathbf{T_C}(\mathbf{K})$	
MnZn	5.364	39.675	0.994	258.911	0.297	0.000	
MnY	6.196	108.703	2.028	239.583	0.728	4.255	
MnZr	5.893	24.904	0.410	244.244	0.332	0.001	
MnNb	5.677	8.838	0.110	237.434	0.285	0.000	
MnMo	5.555	33.610	0.440	303.727	0.813	7.823	
MnTc	5.484	61.030	0.904	290.267	1.199	18.257	
MnRu	5.451	59.824	1.020	350.714	0.645	3.752	
MnRh	5.479	70.719	1.097	313.688	0.526	1.043	
MnPd	5.547	73.929	1.393	237.002	0.736	4.385	
MnAg	5.658	45.308	1.013	214.767	0.413	0.069	
MnCd	5.775	41.281	1.058	206.990	0.202	0.000	
MnLu	6.033	87.389	1.639	207.485	0.713	3.408	
MnHf	5.850	19.263	0.369	227.288	0.283	0.000	
MnTa	5.682	6.678	0.070	221.811	0.212	0.000	
MnW	5.200	31.369	0.429	286.356	0.794	6.850	
MnRe	5.519	59.526	0.872	296.901	1.204	18.821	
MnOs	5.496	58.265	1.000	320.156	0.742	6.070	
MnIr	5.525	62.048	1.145	293.428	0.481	0.480	
MnPt	5.610	80.117	1.445	221.811	0.735	4.064	
MnAu	5.716	40.738	0.908	183.916	0.456	0.183	
MnHg	5.850	35.083	0.903	121.406	0.475	0.180	
FeCo	5.111	112.538	1.982	323.381	0.752	6.458	
FeNi	5.134	40.093	0.691	325.192	0.387	0.041	
FeCu	5.201	45.871	1.153	283.910	0.285	0.000	
Continued on next page							

Table A.1 – continued from previous page

Compound	a ₀ (a.u.)	$\mathbf{N}(\mathbf{E_F})$ (states/Ry)	$\mathbf{N}(\mathbf{E_F})\mathbf{I_S}$	$\langle \omega \rangle$	λ	$\mathbf{T_C}(\mathbf{K})$		
FeZn	5.319	83.971	2.308	277.209	0.270	0.000		
FeY	6.137	70.646	1.548	256.515	0.288	0.000		
FeZr	5.857	16.021	0.334	261.505	0.154	0.000		
FeNb	5.667	57.531	1.112	254.214	0.626	2.355		
FeMo	5.538	85.710	1.444	325.192	0.941	12.484		
FeTc	5.457	94.451	1.746	310.781	0.907	10.888		
FeRu	5.424	109.951	2.575	375.500	0.494	0.777		
FeRh	5.444	135.619	1.870	335.857	0.467	0.422		
FePd	5.508	42.865	0.887	253.752	0.359	0.008		
FeAg	5.621	52.358	1.264	229.946	0.301	0.000		
FeCd	5.743	195.207	5.442	221.619	0.339	0.002		
FeLu	5.988	47.197	0.953	222.149	0.246	0.000		
FeHf	5.813	13.323	0.275	243.352	0.122	0.000		
FeTa	5.600	51.334	1.062	237.487	0.510	0.633		
FeW	5.563	62.519	0.997	306.594	0.752	6.104		
FeRe	5.495	63.285	1.066	317.884	0.794	7.607		
FeOs	5.467	76.781	1.594	342.783	0.476	0.518		
FeIr	5.490	98.392	2.098	314.166	0.401	0.067		
FePt	5.571	50.248	0.974	237.487	0.444	0.179		
FeHg	5.803	110.516	3.066	129.987	0.896	4.415		
CoNi	5.129	125.919	2.840	316.425	0.400	0.065		
CoCu	5.205	105.478	2.535	276.256	0.399	0.055		
CoZn	5.256	41.087	1.206	269.736	0.130	0.000		
CoY	6.156	28.030	0.591	249.600	0.083	0.000		
	Continued on next page							

Table A.1 – continued from previous page

Compound	a ₀ (a.u.)	$N(E_F)$ (states/Ry)	$\mathbf{N}(\mathbf{E_F})\mathbf{I_S}$	$\langle \omega \rangle$	λ	$\mathbf{T_C}(\mathbf{K})$	
CoZr	5.875	27.860	0.380	254.455	0.392	0.038	
CoNb	5.682	47.055	0.642	247.361	0.688	3.522	
СоМо	5.540	50.027	0.707	316.425	0.547	1.366	
CoTc	5.455	63.482	0.916	302.403	0.761	6.287	
CoRu	5.413	83.228	1.360	365.377	0.457	0.374	
CoRh	5.427	52.245	0.889	326.803	0.299	0.000	
CoPd	5.496	76.163	1.803	246.911	0.363	0.010	
CoAg	5.619	120.625	3.240	223.747	0.365	0.010	
CoCd	5.719	52.003	1.448	215.644	0.092	0.000	
CoLu	5.997	17.878	0.344	216.160	0.079	0.000	
CoHf	5.834	26.489	0.392	236.791	0.306	0.000	
CoTa	5.600	40.956	0.571	231.084	0.538	0.903	
CoW	5.560	47.846	0.642	298.329	0.576	1.777	
CoRe	5.487	60.214	0.881	309.314	0.626	2.868	
CoOs	5.454	62.346	1.034	333.542	0.493	0.676	
CoIr	5.472	36.658	0.606	305.696	0.299	0.000	
CoPt	5.554	59.004	1.173	231.084	0.437	0.148	
CoAu	5.669	66.797	1.756	191.605	0.339	0.002	
CoHg	5.824	37.356	1.124	126.482	0.086	0.000	
NiCu	5.218	36.117	0.752	277.804	0.164	0.000	
NiZn	5.321	0.000	0.000	271.247	0.000	0.000	
NiY	6.243	15.152	0.146	250.998	0.191	0.000	
NiZr	5.941	26.540	0.266	255.881	0.397	0.048	
NiNb	5.719	33.932	0.381	248.747	0.538	0.970	
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Table A.1 – continued from previous page

Compound	a ₀ (a.u.)	$N(E_F)$ (states/Ry)	$\mathbf{N}(\mathbf{E_F})\mathbf{I_S}$	$\langle \omega \rangle$	λ	$\mathbf{T_C}(\mathbf{K})$								
NiMo	5.570	42.665	0.525	318.198	0.400	0.065								
NiTc	5.474	43.155	0.540	304.097	0.557	1.483								
NiRu	5.429	27.951	0.362	367.423	0.236	0.000								
NiRh	5.444	42.237	0.587	328.634	0.253	0.000								
NiPd	5.512	42.248	0.770	248.294	0.320	0.000								
NiAg	5.631	32.684	0.714	225.000	0.096	0.000								
NiCd	5.760	14.160	0.279	216.852	0.050	0.000								
NiLu	6.110	14.421	0.147	217.371	0.156	0.000								
NiHf	5.892	21.727	0.211	238.118	0.298	0.000								
NiTa	6.384	57.032	0.617	232.379	0.229	0.000								
NiW	5.586	37.241	0.414	300.000	0.352	0.006								
NiRe	5.503	35.759	0.408	311.047	0.445	0.239								
NiOs	5.465	33.383	0.450	335.410	0.356	0.009								
NiIr	5.487	30.788	0.426	307.409	0.287	0.000								
NiPt	5.570	42.600	0.663	232.379	0.431	0.126								
NiAu	5.690	28.826	0.596	192.678	0.142	0.000								
NiHg	6.051	8.508	0.104	127.191	0.234	0.000								
CuZn	5.442	4.694	0.051	236.813	0.062	0.000								
CuY	6.404	15.363	0.138	219.135	0.239	0.000								
CuZr	6.054	22.661	0.222	223.398	0.378	0.019								
CuNb	5.806	12.684	0.140	217.169	0.354	0.005								
CuMo	5.640	33.408	0.404	277.804	0.447	0.228								
CuTc	5.535	27.539	0.371	265.493	0.421	0.108								
CuRu	5.500	30.452	0.447	320.780	0.222	0.000								
				Continu	ued on r	Continued on next page								

Table A.1 – continued from previous page

Compound	a ₀ (a.u.)	$\mathbf{N}(\mathbf{E_F})$ (states/Ry)	$\mathbf{N}(\mathbf{E_F})\mathbf{I_S}$	$\langle \omega \rangle$	λ	$\mathbf{T_C}(\mathbf{K})$			
CuRh	5.516	66.913	1.045	286.915	0.360	0.010			
CuPd	5.576	20.016	0.261	216.774	0.112	0.000			
CuAg	5.719	7.340	0.070	196.437	0.072	0.000			
CuCd	5.933	5.634	0.055	189.324	0.056	0.000			
CuLu	6.225	13.019	0.115	189.776	0.210	0.000			
CuHf	6.000	48.727	0.477	207.889	0.585	1.350			
CuTa	5.600	8.615	0.076	202.879	0.216	0.000			
CuW	5.649	34.440	0.358	261.916	0.447	0.213			
CuRe	5.560	19.914	0.275	271.560	0.244	0.000			
CuOs	5.527	17.621	0.229	292.831	0.163	0.000			
CuIr	5.559	57.080	0.829	268.384	0.397	0.050			
CuPt	5.629	39.073	0.501	202.879	0.228	0.000			
CuAu	5.767	8.188	0.072	168.219	0.119	0.000			
CuHg	5.957	6.292	0.055	111.044	0.296	0.000			
ZnY	6.598	53.452	0.541	213.963	0.664	2.616			
ZnZr	6.176	10.682	0.115	218.125	0.193	0.000			
ZnNb	5.919	32.374	0.422	212.044	0.753	4.238			
ZnMo	5.746	23.433	0.365	271.247	0.220	0.000			
ZnTc	5.647	24.473	0.412	259.227	0.256	0.000			
ZnRu	5.610	42.842	0.771	313.209	0.150	0.000			
ZnRh	5.604	18.103	0.302	280.143	0.089	0.000			
ZnPd	5.676	8.278	0.095	211.658	0.108	0.000			
ZnAg	5.905	5.246	0.054	191.801	0.078	0.000			
ZnCd	6.206	10.234	0.119	184.855	0.077	0.000			
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Table A.1 – continued from previous page

Compound	a ₀ (a.u.)	$\mathbf{N}(\mathbf{E_F})$ (states/Ry)	$\mathbf{N}(\mathbf{E_F})\mathbf{I_S}$	$\langle \omega \rangle$	λ	$\mathbf{T_C}(\mathbf{K})$		
ZnLu	6.418	21.178	0.194	185.297	0.323	0.000		
ZnHf	6.102	8.154	0.086	202.983	0.108	0.000		
ZnTa	5.900	23.158	0.305	198.091	0.467	0.251		
ZnW	5.754	21.258	0.293	255.734	0.187	0.000		
ZnRe	5.671	20.413	0.297	265.151	0.167	0.000		
ZnOs	5.650	38.534	0.632	285.920	0.162	0.000		
ZnIr	5.661	27.011	0.448	262.050	0.094	0.000		
ZnPt	5.738	13.483	0.176	198.091	0.131	0.000		
ZnAu	5.909	6.824	0.061	164.248	0.179	0.000		
ZnHg	6.382	8.825	0.083	108.423	0.655	1.245		
YZr	6.924	43.198	0.383	201.842	0.570	1.125		
YNb	6.627	41.399	0.401	196.214	0.802	4.838		
YMo	6.462	63.727	0.745	250.998	0.676	3.322		
YTc	6.361	46.012	0.546	239.875	0.454	0.230		
YRu	6.311	19.232	0.188	289.828	0.191	0.000		
YRh	6.364	15.227	0.160	259.230	0.101	0.000		
YPd	6.520	13.587	0.106	195.857	0.191	0.000		
YAg	6.710	17.576	0.151	177.482	0.228	0.000		
YCd	6.924	27.855	0.257	171.056	0.283	0.000		
YLu	7.221	55.027	0.452	171.464	0.590	1.173		
YHf	6.892	48.542	0.414	187.830	0.605	1.469		
YTa	6.654	47.071	0.426	183.303	0.805	4.576		
YW	6.513	60.677	0.615	236.643	0.672	3.053		
YRe	6.417	50.919	0.583	245.357	0.424	0.110		
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Table A.1 – continued from previous page

Compound	a ₀ (a.u.)	$N(E_F)$ (states/Ry)	$\mathbf{N}(\mathbf{E_F})\mathbf{I_S}$	$\langle \omega \rangle$	λ	$\mathbf{T_C}(\mathbf{K})$			
YOs	6.376	50.030	0.686	264.575	0.219	0.000			
YIr	6.408	12.338	0.151	242.487	0.034	0.000			
YPt	6.533	11.974	0.088	183.303	0.174	0.000			
YAu	6.698	15.066	0.118	151.987	0.234	0.000			
YHg	6.914	23.090	0.202	100.329	0.629	0.958			
ZrNb	6.349	56.839	0.484	200.031	1.604	18.939			
ZrMo	6.189	45.227	0.411	255.881	0.842	7.313			
ZrTc	6.102	21.994	0.220	244.541	0.406	0.062			
ZrRu	6.073	7.295	0.060	295.466	0.148	0.000			
ZrRh	6.120	22.778	0.208	264.273	0.339	0.002			
ZrPd	6.229	62.403	0.757	199.667	0.874	6.335			
ZrAg	6.371	40.777	0.435	180.935	0.524	0.588			
ZrCd	6.507	4.177	0.045	174.383	0.051	0.000			
ZrLu	6.786	40.978	0.358	174.800	0.601	1.323			
ZrHf	6.564	47.514	0.391	191.484	0.841	5.449			
ZrTa	6.363	58.371	0.476	186.869	1.447	15.581			
ZrW	6.223	39.349	0.340	241.247	0.721	4.126			
ZrRe	6.149	15.390	0.133	250.130	0.261	0.000			
ZrOs	6.118	6.080	0.046	269.722	0.140	0.000			
ZrIr	6.165	22.527	0.205	247.204	0.314	0.000			
ZrPt	6.263	28.732	0.257	186.869	0.512	0.508			
ZrAu	6.388	34.183	0.336	154.944	0.609	1.259			
ZrHg	6.580	4.957	0.059	102.281	0.138	0.000			
NbMo	5.995	15.108	0.129	248.747	0.415	0.084			
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Table A.1 – continued from previous page

Compound	a ₀ (a.u.)	$N(E_F)$ (states/Ry)	$\mathbf{N}(\mathbf{E_F})\mathbf{I_S}$	$\langle \omega \rangle$	λ	$\mathbf{T_C}(\mathbf{K})$
NbTc	5.926	8.813	0.072	237.724	0.322	0.000
NbRu	5.904	44.338	0.464	287.228	0.739	5.370
NbRh	5.942	45.685	0.468	256.905	0.827	6.962
NbPd	6.016	32.143	0.339	194.100	0.675	2.547
NbAg	6.135	23.780	0.272	175.891	0.454	0.167
NbCd	6.253	25.453	0.374	169.521	0.406	0.044
NbLu	6.492	38.583	0.360	169.926	0.877	5.451
NbHf	6.318	57.764	0.478	186.145	1.528	16.637
Nb Ta	6.143	32.190	0.265	181.659	1.068	9.235
Nb W	6.023	12.647	0.098	234.521	0.350	0.004
NbRe	5.972	7.499	0.059	243.156	0.237	0.000
NbOs	5.955	31.674	0.312	262.202	0.665	3.233
NbIr	5.994	39.837	0.390	240.312	0.752	4.792
NbPt	6.061	41.104	0.425	181.659	0.879	5.865
NbAu	6.167	21.967	0.247	150.624	0.499	0.338
NbHg	6.265	31.192	0.435	99.430	1.112	5.465
MoTc	5.817	29.159	0.303	304.097	0.666	3.775
MoRu	5.797	72.200	0.818	367.423	0.551	1.669
MoRh	5.819	42.076	0.462	328.634	0.401	0.071
MoPd	5.879	41.556	0.471	248.294	0.559	1.240
MoAg	5.990	30.624	0.399	225.000	0.383	0.023
MoCd	6.099	26.941	0.429	216.852	0.197	0.000
MoLu	6.321	54.804	0.619	217.371	0.723	3.760
MoHf	6.156	46.447	0.415	238.118	0.725	4.157
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Table A.1 – continued from previous page

Compound	a ₀ (a.u.)	$\mathbf{N}(\mathbf{E_F})$ (states/Ry)	$\mathbf{N}(\mathbf{E_F})\mathbf{I_S}$	$\langle \omega \rangle$	λ	$\mathbf{T_C}(\mathbf{K})$			
МоТа	6.000	13.521	0.112	232.379	0.296	0.000			
MoW	5.916	14.228	0.132	300.000	0.257	0.000			
MoRe	5.857	24.930	0.247	311.047	0.477	0.475			
MoOs	5.842	50.208	0.530	335.410	0.549	1.495			
MoIr	5.872	52.861	0.556	307.409	0.528	1.051			
MoPt	5.932	49.517	0.542	232.379	0.706	3.673			
MoAu	6.020	37.591	0.470	192.678	0.636	1.935			
MoHg	6.126	22.320	0.336	127.191	0.684	1.764			
TcRu	5.720	51.252	0.588	351.141	0.458	0.367			
TcRh	5.737	47.970	0.535	314.070	0.512	0.858			
TcPd	5.785	41.566	0.510	237.291	0.657	2.773			
TcAg	5.880	27.332	0.394	215.029	0.363	0.009			
TcCd	5.986	25.079	0.422	207.243	0.208	0.000			
TcLu	6.216	44.542	0.569	207.738	0.482	0.350			
TcHf	6.063	18.513	0.180	227.565	0.293	0.000			
ТсТа	5.932	7.043	0.056	222.081	0.209	0.000			
TcW	5.837	22.790	0.225	286.705	0.520	0.875			
TcRe	5.790	35.922	0.370	297.263	0.657	3.469			
TcOs	5.769	42.057	0.457	320.546	0.458	0.337			
TcIr	5.800	46.495	0.507	293.786	0.396	0.053			
TcPt	5.846	51.275	0.577	222.081	0.665	2.741			
TcAu	5.928	26.349	0.348	184.140	0.486	0.333			
TcHg	6.047	20.252	0.332	121.554	0.590	0.829			
RuRh	5.700	75.610	0.899	379.473	0.357	0.011			
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Table A.1 – continued from previous page

Compound	a ₀ (a.u.)	$\mathbf{N}(\mathbf{E_F})$ (states/Ry)	$\mathbf{N}(\mathbf{E_F})\mathbf{I_S}$	$\langle \omega \rangle$	λ	$\mathbf{T_C}(\mathbf{K})$	
RuPd	5.741	26.917	0.332	286.705	0.319	0.000	
RuAg	5.828	35.729	0.554	259.808	0.313	0.000	
RuCd	6.003	142.275	2.718	250.400	0.391	0.037	
RuLu	6.172	41.420	0.486	250.998	0.209	0.000	
RuHf	6.034	4.838	0.036	274.955	0.103	0.000	
RuTa	5.911	46.653	0.496	268.328	0.618	2.339	
RuW	5.821	55.931	0.612	346.410	0.439	0.232	
RuRe	5.762	62.290	0.775	359.166	0.395	0.062	
RuOs	5.743	44.128	0.505	387.298	0.238	0.000	
RuIr	5.764	92.439	1.112	354.965	0.326	0.001	
RuPt	5.807	31.743	0.382	268.328	0.366	0.012	
RuAu	5.893	26.850	0.399	222.486	0.333	0.001	
RuHg	6.038	29.902	0.512	146.867	0.661	1.755	
RhPd	5.754	63.456	1.007	256.437	0.290	0.000	
\mathbf{RhAg}	5.866	70.639	1.170	232.379	0.344	0.003	
RhCd	5.976	0.000	0.292	223.964	0.072	0.000	
RhLu	6.216	12.434	0.128	224.499	0.093	0.000	
RhHf	6.076	23.393	0.215	245.927	0.303	0.000	
Rh Ta	5.943	39.103	0.373	240.000	0.646	2.591	
Rh W	5.836	41.136	0.411	309.839	0.396	0.055	
RhRe	5.774	48.305	0.505	321.248	0.419	0.124	
RhOs	5.743	64.241	0.725	346.410	0.374	0.025	
RhIr	5.757	36.272	0.410	317.490	0.224	0.000	
RhPt	5.813	36.515	0.439	240.000	0.349	0.004	
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Table A.1 – continued from previous page

Compound	a ₀ (a.u.)	$\mathbf{N}(\mathbf{E_F})$ (states/Ry)	$\mathbf{N}(\mathbf{E_F})\mathbf{I_S}$	$\langle \omega \rangle$	λ	$\mathbf{T_C}(\mathbf{K})$
RhAu	5.907	63.207	1.060	198.997	0.394	0.033
RhHg	6.061	32.864	0.619	131.362	0.199	0.000
PdAg	5.918	9.590	0.092	175.571	0.086	0.000
PdCd	5.991	0.000	0.000	169.213	0.000	0.000
PdLu	6.370	12.291	0.095	169.617	0.170	0.000
PdHf	6.183	24.259	0.215	185.806	0.403	0.043
PdTa	6.008	32.445	0.308	181.328	0.651	2.034
PdW	5.892	42.005	0.421	234.094	0.629	2.223
PdRe	5.816	36.019	0.385	242.714	0.602	1.841
PdOs	5.778	24.092	0.244	261.725	0.362	0.010
PdIr	5.796	31.318	0.361	239.875	0.354	0.006
PdPt	5.852	28.945	0.325	181.328	0.468	0.232
PdAu	5.963	17.190	0.204	150.350	0.172	0.000
PdHg	6.149	11.928	0.116	99.249	0.299	0.000
AgCd	6.205	5.090	0.047	153.338	0.074	0.000
AgLu	6.570	14.581	0.120	153.704	0.179	0.000
AgHf	6.314	40.274	0.390	168.375	0.545	0.711
AgTa	6.000	10.459	0.100	164.317	0.211	0.000
AgW	5.982	33.386	0.372	212.132	0.438	0.138
AgRe	5.893	26.886	0.315	219.943	0.377	0.018
AgOs	5.866	28.891	0.459	237.171	0.270	0.000
AgIr	5.897	46.869	0.641	217.371	0.511	0.584
AgPt	5.994	7.835	0.079	164.317	0.093	0.000
AgAu	6.061	7.416	0.052	136.244	0.108	0.000
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Table A.1 – continued from previous page

Compound	a ₀ (a.u.)	$N(E_F)$ (states/Ry)	$\mathbf{N}(\mathbf{E_F})\mathbf{I_S}$	$\langle \omega \rangle$	λ	$\mathbf{T_C}(\mathbf{K})$
AgHg	6.286	6.293	0.053	89.937	0.313	0.000
CdLu	6.761	20.147	0.181	148.138	0.213	0.000
CdHf	6.445	7.756	0.083	162.278	0.074	0.000
CdTa	6.245	27.503	0.359	158.367	0.408	0.044
CdW	6.099	23.161	0.286	204.450	0.184	0.000
CdRe	6.015	20.504	0.308	211.979	0.153	0.000
CdOs	5.998	63.051	0.949	228.583	0.237	0.000
CdIr	6.027	24.058	0.398	209.499	0.076	0.000
CdPt	6.073	11.058	0.134	158.367	0.076	0.000
CdAu	6.275	6.346	0.050	131.311	0.093	0.000
CdHg	6.673	9.860	0.095	86.681	0.462	0.098
LuHf	6.751	0.000	0.000	162.665	0.000	0.000
LuTa	6.516	46.678	0.409	158.745	0.853	4.705
LuW	6.349	15.187	0.188	204.939	0.133	0.000
LuRe	6.249	43.962	0.478	212.485	0.422	0.089
LuOs	6.254	31.672	0.367	229.129	0.220	0.000
LuIr	6.246	9.407	0.128	210.000	0.036	0.000
LuPt	6.387	0.000	0.000	158.745	0.000	0.000
LuAu	6.568	13.672	0.111	131.624	0.215	0.000
LuHg	6.764	16.915	0.145	86.888	0.552	0.398
HfTa	6.324	51.626	0.415	173.897	1.141	10.034
HfW	6.180	39.569	0.337	224.499	0.575	1.325
HfRe	6.103	18.496	0.173	232.766	0.219	0.000
HfOs	6.073	4.445	0.031	250.998	0.088	0.000
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Table A.1 – continued from previous page

Compound	a ₀ (a.u.)	$\mathbf{N}(\mathbf{E_F})$ (states/Ry)	$\mathbf{N}(\mathbf{E_F})\mathbf{I_S}$	$\langle \omega \rangle$	λ	$\mathbf{T_C}(\mathbf{K})$
HfIr	6.119	22.415	0.206	230.043	0.261	0.000
HfPt	6.207	21.411	0.186	173.897	0.373	0.011
HfAu	6.330	24.349	0.202	144.187	0.555	0.689
HfHg	6.472	3.784	0.037	95.181	0.124	0.000
TaW	6.025	22.052	0.196	219.089	0.403	0.051
TaRe	5.971	7.105	0.057	227.156	0.172	0.000
TaOs	5.959	41.874	0.409	244.949	0.559	1.217
TaIr	5.994	28.684	0.263	224.499	0.436	0.141
TaPt	6.056	36.571	0.351	169.706	0.748	3.327
TaAu	6.151	15.854	0.158	140.712	0.341	0.001
TaHg	6.887	30.910	0.417	92.887	0.706	1.462
WRe	5.877	19.919	0.190	293.258	0.347	0.004
WOs	5.871	41.897	0.423	316.228	0.415	0.109
WIr	5.897	50.015	0.491	289.828	0.488	0.543
WPt	5.953	38.597	0.381	219.089	0.579	1.345
WAu	6.029	37.559	0.414	181.659	0.709	2.918
WHg	6.145	24.198	0.342	119.917	0.889	3.990
ReOs	5.813	35.740	0.369	327.872	0.295	0.000
ReIr	5.835	48.779	0.499	300.500	0.357	0.009
RePt	5.874	46.170	0.450	227.156	0.653	2.571
ReAu	5.940	19.168	0.258	188.348	0.376	0.015
ReHg	6.050	16.550	0.243	124.332	0.651	1.396
OsIr	5.810	72.169	0.817	324.037	0.347	0.005
OsPt	5.842	30.353	0.297	244.949	0.431	0.134
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Table A.1 – continued from previous page

Compound	a ₀ (a.u.)	$\mathbf{N}(\mathbf{E_F})$ (states/Ry)	$\mathbf{N}(\mathbf{E_F})\mathbf{I_S}$	$\langle \omega \rangle$	λ	$\mathbf{T_C}(\mathbf{K})$
OsAu	5.911	26.142	0.307	203.101	0.863	6.234
OsHg	6.076	56.481	0.930	134.071	1.569	12.364
IrPt	5.856	73.165	0.860	224.499	0.335	0.001
IrAu	5.939	47.942	0.718	186.145	0.417	0.068
IrHg	6.065	31.834	0.524	122.878	0.358	0.004
PtAu	5.994	18.262	0.203	140.712	0.211	0.000
PtHg	6.178	9.856	0.107	92.887	0.206	0.000
AuHg	6.284	9.376	0.082	77.018	0.425	0.035

Table A.1 – continued from previous page

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BIOGRAPHY

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