Crystal Structures and Electronic Properties of BaAu Compound under High Pressure

Bingtan Li 1, Jiayun Wang 1,*, Shuai Sun 2,* and Hanyu Liu 1

1 State Key Laboratory of Superhard Materials, International Center of Computational Method & Software, College of Physics, Jilin University, Changchun 130012, China
2 Engineering Training Center, Jilin University, Changchun 130012, China
* Correspondence: wangjianyun@jlu.edu.cn (J.W.); ss88311@jlu.edu.cn (S.S.)

Abstract: The investigations of Au-bearing alloy materials have been of broad research interest as their relevant features exhibit significant advantages compared with pure Au. Here, we extensively investigate the compression behaviors of BaAu compounds via first-principles calculations and find that a high-pressure cubic phase is calculated to be stable above 12 GPa. Further electronic calculations indicate that despite the low electronegativity of Ba, \( Fd-3m \)-structured BaAu exhibits metallic characteristics, which is different from those of semiconducting alkali metal aurides that possess slight characteristics of an ionic compound. These findings provide a step toward a further understanding of the electronic properties of BaAu compounds and provide key insight for exploring the other Au-bearing alloy materials under extreme conditions.

Keywords: Au-bearing alloy; high pressure; first-principles calculation

1. Introduction

Gold (Au), one of the most well-known precious metals, has attracted significant interest due to its chemical inertness and fascinating physical properties under normal conditions [1–7]. Furthermore, it has been found that Au could react with other elements and form plenty of aurides with diverse applications such as catalysis, electronic transport, and optics [8–11]. Among them, Au-based alloys have become an important family of materials because of their excellent performances, superior to pure Au. For instance, the economic cost and stability are simultaneously balanced in Au-Cu alloys [12–14]; superconductivity that is inaccessible in Au has been observed in Au-In and Au-Pb alloys [15–17]; Au and Li atoms can form unexpected stoichiometric intermetallic compounds at high pressure, where Au obtains electrons from Li and behaves as a \( p \)-block element [18]. Therefore, it is of great interest to further investigate new gold-based alloy materials that may possess remarkable properties.

It is worth mentioning that some alkali metal aurides, including KAu, RbAu, and CsAu, are semiconductors [19–22], whose bandgaps range from 0.1 eV for KAu to 1.0 eV for CsAu crystallizing in a CsCl-type structure [20], albeit the fact that all the constituent elements are typical metals. This anomaly can be understood as alkali metals with relatively low electronegativities dramatically donating valence electrons to Au and showing ionic-compound-like features in the forming compounds. Compared to alkali-metal elements, alkaline earth metals have similar low electronegativity, ionic radii, and -6 s orbital energy [23–25]. Among alkaline earth metals, Ba has the lowest electronegativity based on the Pauling scale, which indicates that it is easy to lose electrons and tends to become a cation once its compound forms [25]. Previous studies [26] indicate that the BaAu compound was stabilized with \( Pnma \) symmetry at atmospheric pressure, which is also theoretically suggested in our recent study [27]. However, the ground-state \( Pnma \)-structured BaAu is still metallic material under ambient conditions [28].
Moreover, it has been recognized that pressure is an effective tool to shorten chemical bonds and reconstruct atomic arrangements, thus inducing a crystal structure phase transition and the appearance of novel electronic structures inaccessible at atmospheric pressure [29–35]. For instance, the typical alkali Na metal has been experimentally proven to become a transparent insulator with a large bandgap under high pressure due to the p-d orbital hybridization of shell electrons and the electron localization in atomic interstices [36]. The compressed NiTi intermetallic compound is proposed to be a semiconducting state associated with its unique band structure and the nature of 3d orbitals localization [37]. As a consequence, it is an open question to explore whether a similar property could appear in any other system other than alkali metal aurides and whether BaAu could be a semiconductor under high-pressure.

In this work, therefore, we systematically conduct a theoretical investigation of stoichiometric BaAu and its related electronic properties under high pressure. Our first-principles calculations reveal that the compressed BaAu compound is still metallic below megabar pressure as only part of the valence electrons of Ba are transformed to Au, and the residual ones are still cruising electrons. These findings uncover the high-pressure properties of the BaAu intermetallic compound and provide key insights for exploring the other Au-bearing alloy materials under extreme conditions.

2. Computational Details

First-principles calculations, including total energy calculations, structural relaxations, electronic structures, and phonon dispersions for the BaAu structures under different pressures, were performed using the projector augmented-wave [38] method in the Vienna Ab initio Simulation Package (VASP) code Version 6.1.0 [39]. The Perdew–Burke–Ernzerhof (PBE) [40] in the generalized gradient approximation (GGA) was used to describe the exchange-correlational functional [41]. The electron–ion interactions were represented by pseudopotentials built within the scalar relativistic projector augmented wave method with 5s25p66s2 and 5d106s1 valence electrons for Ba and Au atoms, respectively. A plane-wave kinetic energy cutoff of 600 eV and dense k-point sampling (2π × 0.03 Å⁻¹) was shown to give an excellent convergence of energies. The electron localization function (ELF) [42,43] was also calculated using VASP code. The dynamical stabilities of the ground-state structures at varying pressures were determined by using the density functional perturbation theory (DFPT) [44] as implemented in the Phonopy code [45–47] with a 600 eV energy cutoff. A 2 × 3 × 2 supercell with 96 atoms and a 3 × 3 × 3 supercell with 108 atoms were used to calculate the phonon dispersions for an ambient Pnma-BaAu structure and high-pressure Fd-3m-BaAu under high pressure, respectively. In this process, force was calculated with a threshold of 1 × 10⁻⁷ eV/Å. The schematic figure of this manuscript was shown in Figure 1.

![Figure 1](image_url)

Figure 1. The schematic figure of this manuscript.
3. Results and Discussion

To study the thermodynamic stability of intermetallic compound BaAu at high pressure, AB-type prototypes of binary Au-bearing compounds selected from the Open Quantum Materials Database (OQMD) [48,49] were chosen as candidate structures. The enthalpies of these structures were calculated as a function of the external pressure and plotted relative to the enthalpy of the ambient \( Pnma \)-BaAu structure, as shown in Figure 2a. Under a pressure range from 0 to 12 GPa, \( Pnma \)-BaAu was the lowest-energy structure. At elevated pressures above 12 GPa, the \( Fd-3m \) structure became energetically more favorable than \( Pnma \)-BaAu; therefore, the \( Pnma \)-BaAu transformed into \( Fd-3m \)-BaAu at high pressure. At atmospheric pressure, the lattice parameter of \( a/b \) and \( a/c \) was ~1.69 and 1.30, respectively. Under high pressure, the \( Pnma \)-BaAu was drastically compressed, the lattice parameter of \( a \) and \( c \) showed a rapid decrease, and a structural phase transition occurred at ~12 GPa, when the \( Pnma \)-BaAu structure transformed into a cubic structure with \( Fd-3m \) symmetry. This high-pressure \( Fd-3m \) phase consisted of two interpenetrating \( \{BaAu_4\} \) and \( \{Ba_4Au\} \) tetrahedra (Figure 2b), whose lattice parameters and atomic coordinates are listed in Table 1. Table S1 gives detailed structural information of other BaAu compounds in the Supplementary Materials. The phonon dispersion spectra of ambient and high-pressure structures were simulated based on density functional perturbation theory (Figure 2c,d), where there is no imaginary phonon mode in the first Brillouin zones. These results confirmed the dynamical stability of these two phases.

![Figure 2](image-url)

Figure 2. (a) Enthalpy as a function of external pressure for selected structures of BaAu in different symmetries. (b) The crystal structure of the \( Fd-3m \) BaAu under high pressure. Yellow and red spheres represent Ba and Au atoms, respectively. Phonon dispersions of BaAu with (c) \( Pnma \) symmetry at 10 GPa and (d) \( Fd-3m \) symmetry at 25 GPa.
Table 1. Structural parameters of stable BaAu compounds under high pressure.

| Compound | Pressure (GPa) | Space Group | Lattice Parameter (Å) | Atomic Coordinate (Fractional) |
|----------|----------------|-------------|-----------------------|-------------------------------|
|          |                |             |                       |                               |
| BaAu     | 10             | Pnma        | \(a = 7.922\) \(b = 4.705\) \(c = 6.087\) \(\alpha = \beta = \gamma = 90\) | Ba 0.317 0.750 0.136          |
|          | 25             | Fd-3m       | \(a = b = c = 7.034\) \(\alpha = \beta = \gamma = 90\) | Au 0.040 0.250 0.136          |

To provide insights into the nature of the chemical bonding of the BaAu compounds, we calculated the projected density of states (PDOS) of the stable phases at 10 (a), 25 (b), and 100 GPa (c). In Figure 3b,c, Fd-3m-BaAu showed a significant Au 5d component below the Fermi level. By analyzing the electronic states around the Fermi level, we found considerable overlap between Ba 5d and Au 6p orbits, indicating that the charge transfer and the components participated in the Ba-Au bonding. Furthermore, a hypothetical model system of Ba\(_0\)Au was constructed, in which all the Ba atoms were removed from the high-pressure Fd-3m-BaAu structure. The calculated PDOS of Ba\(_0\)Au is plotted in Figure 3d. The absence of 6p electrons in the hypothetical Ba\(_0\)Au structure confirmed that Au 6p orbital gained electrons from Ba in BaAu compounds. These results also indicated that the Ba 5d orbital had a higher energy relative to Ba 6s under current pressure, which has been demonstrated in previous studies [23]. In addition, the calculated PDOS of BaAu in the Pnma structure is shown in Figure 3a. The structure of orthorhombic Pnma-BaAu showed metallic characteristics at 10 GPa.

![Figure 3](image-url)

**Figure 3.** (a) PDOS calculated using the Perdew–Burke–Ernzerhof functional for BaAu in the Pnma structure at 10 GPa. PDOS calculated for BaAu in the Fd-3m structure at (b) 25 GPa, (c) 100 GPa, and (d) hypothetical Ba\(_0\)Au at 25 GPa. The dashed line at zero indicates the Fermi energy.
Moreover, we calculated the electron localization function (ELF) to investigate the chemical bonding in the crystal structure of BaAu under high pressure. As shown in Figure 4a, the low values between Ba and Au atoms showed the ionic bonding feature of Ba-Au bonds, implying the charge transfer between Ba and Au atoms. To further illustrate the charge transfer between Ba and Au atoms, we performed Bader charge analysis on BaAu compounds. As shown in Figure 4b, it is obvious that the Bader charge on Au decreased with increasing pressure. The Bader charge on Au demonstrates a Ba$^{1+}$ oxidation state in high-pressure BaAu compounds. The accepted charges from Ba mainly filled the 6s and 6p orbitals of Au, which plays an important role in stabilizing BaAu compounds under pressure. Moreover, considering the bond length of Ba-Au bonds in Fd-$3m$-BaAu compounds, the interaction between Ba and Au atoms was examined by calculating the integrated crystal orbital Hamilton populations (ICOHP), which can be scaled with the bond strength in compounds by counting the energy-weighted population of wavefunctions between two atomic orbitals. The calculated ICOHP of Ba-Au bonds were $-0.18$ and $-0.17$ eV per pair in BaAu compounds at 25 and 100 GPa, respectively, indicating the strengthening of Ba-Au interactions.

As shown in Figure 3, there was no band gap in the PDOS of the $Pnma$ or Fd-$3m$-structured BaAu compounds, which means that the BaAu compounds showed metallic characteristics in the pressure range from 0 to 100 GPa. We further calculated the PDOS of BaAu and CsAu with the CsCl-type structure at ambient pressure and plotted them in Figure 5. Compared with the PDOS of CsAu, the Fermi level of BaAu had a significant upward shift, which caused the Fermi level to pass through the conduction bands and made BaAu show metal characteristics. The movement of the Fermi level was caused by the extra electron introduced from Ba when replacing the Cs element with Ba, which is equivalent to doping electrons. We also performed Bader charge analysis on the CsAu and BaAu compounds. We found that the Au atoms in CsCl-type CsAu and BaAu gained 0.76 and 1.20 $e$ at zero pressure, respectively. Considering that Bader charge analysis often underestimates the charge transfers for ionic compounds, we believe that the electron on the 6s orbital of Cs atoms was fully transferred and Au atoms had a full-shell structure in the CsAu compound. In contrast, the Au atoms gained more than one electron from Ba atoms and acted as $p$-block elements in the BaAu compound, which can be seen in Figure 5b. These results offer an understandable explanation for the different electronic properties of CsAu and BaAu compounds.
Figure 5. PDOS calculated for CsAu (a) and BaAu (b) with the CsCl-type structure at 0 GPa.

4. Conclusions

In summary, we investigated the stabilities, crystal structures, and electron properties of BaAu compounds under pressure by using first-principles calculations. BaAu exhibited metal characteristics under the pressure range of 0–100 GPa. Detailed analysis of the electronic properties showed that the electronic configurations of elements played key roles in determining the electronic properties of gold-bearing compounds. These findings offer a reasonable explanation for the metallic characteristics of BaAu compounds under high pressure and may represent a step forward in understanding the electronic properties of aurides.

Supplementary Materials: The following are available online at https://www.mdpi.com/article/10.3390/ma15207381/s1, Table S1: Structural parameters of other BaAu compounds at atmospheric pressure; Figure S1: Calculated electron localization function (ELF) for Pnma-BaAu compounds at 0 GPa; Figure S2: Phonon dispersions of BaAu with Fd-3m symmetry at 100 GPa.

Author Contributions: Conceptualization, B.L.; writing—original draft preparation, B.L.; investigation, B.L., J.W., S.S. and H.L. All authors have read and agreed to the published version of the manuscript.

Funding: Fundamental Research Funds for the Central Universities and the Program for Jilin University Science and Technology Innovative Research Team (JLUSTIRT).

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Data sharing is not applicable to this article.

Acknowledgments: B.L. and H.L. acknowledge the Facility of High-Performance Computing Center of Jilin University.

Conflicts of Interest: The authors declare no conflict of interest.

References
1. Hutchings, G.J.; Brust, M.; Schmidbaur, H. Gold—An introductory perspective. Chem. Soc. Rev. 2008, 37, 1759–1765. [CrossRef]
2. Lin, J.; Zhang, S.; Wei, G.; Yang, G.; Ma, Y. Gold with +4 and +6 Oxidation States in AuF$_4$ and AuF$_6$. J. Am. Chem. Soc. 2018, 140, 9545–9550. [CrossRef]
3. Qin, Z.; Bischof, J.C. Thermophysical and biological responses of gold nanoparticle laser heating. Chem. Soc. Rev. 2012, 41, 1191–1217. [CrossRef] [PubMed]
4. Yang, X.; Yang, M.; Pang, B.; Vara, M.; Xia, Y. Gold nanomaterials at work in biomedicine. Chem. Rev. 2015, 115, 10410–10488. [CrossRef] [PubMed]
5. Gimeno, M.C.; Laguna, A. Some recent highlights in gold chemistry. Gold Bull. 2003, 36, 83–92. [CrossRef]
6. Jansen, M. The chemistry of gold as an anion. Chem. Soc. Rev. 2008, 37, 1826–1835. [CrossRef] [PubMed]
7. Pyykö, P. Theoretical chemistry of gold. II. Inorg. Chim. Acta 2005, 358, 4113–4130. [CrossRef]
8. Guenther, J.; Mallet-Ladeira, S.; Estevez, L.; Miqueu, K.; Angoume, A.; Bourissou, D. Activation of Aryl Halides at Gold(I): Practical Synthesis of (PC) Cyclometalated Gold(III) Complexes. J. Am. Chem. Soc. 2014, 136, 1778–1781. [CrossRef]

9. Rudolph, M.; Hashmi, A.S.K. Gold catalysis in total synthesis—An update. Chem. Soc. Rev. 2012, 41, 2448–2462. [CrossRef]

10. Kodiyath, R.; Manikandan, M.; Liu, L.; Ramesh, C.V.; Koyasu, S.; Miyauchi, M.; Sakuma, Y.; Tanabe, T.; Gunji, T.; Diao, T.D.; et al. Visible-light photodecomposition of acetaldehyde by TiO$_2$-coated gold nanocages: Plasmon-mediated hot electron transport via defect states. Chem. Commun. 2014, 50, 15553–15556. [CrossRef]

11. Aragoni, M.C.; Arca, M.; Devillanova, F.A.; Isaia, F.; Lippolis, V.; Pintus, A. Gold(III) Complexes of Asymmetrically Aryl-Substituted 1,2-Dithiolate Ligands Featuring Potential-Controlled Spectroscopic Properties: An Insight into the Electronic Properties of bis(Pyren-1-yl-ethylen-1,2-dithiolato) Gold(III). Chem. -Asian J. 2011, 6, 198–208. [CrossRef]

12. Motl, N.E.; Ewusi-Annan, E.; Sines, I.T.; Jensen, L.; Schaar, R.E. Au—Cu Alloy Nanoparticles with Tunable Compositions and Plasmonic Properties: Experimental Determination of Composition and Correlation with Theory. J. Phys. Chem. C 2010, 114, 19263–19269. [CrossRef]

13. Liu, X.; Wang, A.; Zhang, T.; Su, D.-S.; Mou, C.-Y. Au–Cu alloy nanoparticles supported on silica gel as catalyst for CO oxidation: Effects of Au/Cu ratios. Catal. Today 2011, 160, 103–108. [CrossRef]

14. Zhao, W.; Yang, L.; Yin, Y.; Jin, M. Thermodynamic controlled synthesis of intermetallic Au$_3$Cu alloy nanocrystals from Cu microparticles. J. Mater. Chem. A 2014, 2, 902–906. [CrossRef]

15. Buchal, C.; Mueller, R.M.; Pobell, F.; Kubota, M.; Folke, H.R. Superconductivity investigations of Au-In alloys and of Au at ultralow temperatures. Solid State Commun. 1982, 42, 43–47. [CrossRef]

16. Baranov, D.S.; Vlaic, S.; Baptista, J.; Cofler, E.; Stolyarov, V.S.; Roditchev, D.; Pons, S. Gold Atoms Promote Macroscopic Superconductivity in an Atomic Monolayer of Pb on Si(111). Nano Lett. 2022, 22, 652–657. [CrossRef]

17. Xing, Y.; Wang, H.; Li, C.K.; Zhang, X.; Liu, J.; Zhang, Y.; Luo, J.; Wang, Z.; Wang, Y.; Ling, L.; et al. Superconductivity in topologically nontrivial material Au$_2$Pb. NPJ Quantum Mater. 2016, 1, 1–8. [CrossRef]

18. Yang, G.; Wang, Y.; Peng, F.; Bergara, A.; Ma, Y. Gold as a 6p-Element in Dense Lithium Aurides. J. Am. Chem. Soc. 2016, 138, 4046–4052. [CrossRef]

19. Koenig, C.; Christensen, N.E.; Kollar, J. Electronic properties of alkali-metal—Gold compounds. Phys. Rev. B 1984, 29, 6481. [CrossRef]

20. Miao, M.; Brgoch, J.; Krishnapriyan, A.; Goldman, A.; Kurzman, J.A.; Seshadri, R. On the Stereoelectronic Inertness of the Auride Lone Pair: Ab initio Studies of AAu (A = K, Rb, Cs). Inorg. Chem. 2013, 52, 8183–8189. [CrossRef]

21. Aycibin, M.; Dogan, E.K.; Gulebaglan, S.E.; Secuk, M.N.; Erdinc, B.; Akkus, H. Physical properties of RbAu compound. Comput. Condens. Matter 2014, 1, 32–37. [CrossRef]

22. Spencer, W.E.; Sommer, A.H.; White, J.G. Studies of the Semiconducting Properties of RbAu compound. Phys. Rev. 1959, 115, 57. [CrossRef]

23. Li, F.; Zhang, X.; Fu, Y.; Wang, Y.; Bergara, A.; Yang, G. Ba with Unusual Oxidation States in Ba Chalcogenides under Pressure. J. Phys. Chem. Lett. 2021, 12, 4023–4032. [CrossRef] [PubMed]

24. Luo, D.; Wang, Y.; Yang, G.; Ma, Y. Barium in High Oxidation States in Pressure-Stabilized Barium Fluorides. J. Phys. Chem. C 2018, 122, 12448–12453. [CrossRef]

25. Rahm, M.; Cammi, R.; Ashcroft, N.W.; Hoffmann, R. Squeezing All Elements in the Periodic Table: Electron Configuration and Electronegativity of the Atoms under Compression. J. Am. Chem. Soc. 2019, 141, 10253–10271. [CrossRef] [PubMed]

26. Fornasini, M. New Alkaline Earth Equiatomic Phases: SrAu and BaAu. J. Solid State Chem. 1985, 59, 60–64. [CrossRef]

27. Li, B.; Liu, H.; Liu, G.; Chen, K. First-principles study on high-pressure phases and compression properties of gold-bearing intermetallic compounds. J. Phys. Condens. Matter 2022, 34, 464001–464008. [CrossRef] [PubMed]

28. Munro, J.M.; Latimer, K.; Horton, M.K.; Dwarkanath, S.; Persson, K.A. An improved symmetry-based approach to reciprocal space path selection in band structure calculations. NPJ Comput. Mater. 2020, 6, 1–6. [CrossRef]

29. Zurek, E.; Hoffmann, R.; Ashcroft, N.W.; Oganov, A.R.; Lyakhov, A.O. A little bit of lithium does a lot for hydrogen. Proc. Natl. Acad. Sci. USA 2009, 106, 17640–17643. [CrossRef] [PubMed]

30. Mcmillan, P.F. Chemistry at high pressure. Chem. Soc. Rev. 2006, 35, 855–857. [CrossRef]

31. Peng, F.; Miao, M.; Wang, H.; Li, Q.; Ma, Y. Predicted lithium-boron compounds under high pressure. J. Am. Chem. Soc. 2012, 134, 18599–18605. [CrossRef] [PubMed]

32. Miao, M.; Wang, X.-b; Brgoch, J.; Spera, F.; Jackson, M.G.; Kresse, G.; Lin, H.-q. Anionic Chemistry of Noble Gases: Formation of Mg–NG (NG = Xe, Kr, Ar) Compounds under Pressure. J. Am. Chem. Soc. 2015, 137, 14122–14128. [CrossRef] [PubMed]

33. Zhang, W.; Oganov, A.R.; Goncharov, A.F.; Zhu, Q.; Bouffel, S.E.; Lyakhov, A.O.; Stavrou, E.; Somayazulu, M.; Prakapenka, V.B.; Konopková, Z. Unexpected Stable Stoichiometries of Sodium Chlorides. Science 2013, 342, 1502–1505. [CrossRef] [PubMed]

34. Miao, C. Caesium in high oxidation states and as a p-block element. Nat. Chem. 2013, 5, 846–852. [CrossRef] [PubMed]

35. Zhu, L.; Liu, H.; Pickard, C.J.; Zou, G.; Ma, Y. Reactions of xenon with iron and nickel are predicted in the Earth’s inner core. Nat. Chem. 2014, 6, 644–648. [CrossRef]

36. Ma, Y.; Eremets, M.; Oganov, A.R.; Xie, Y.; Troján, I.; Medvedev, S.; Lyakhov, A.O.; Valle, M.; Prakapenka, V. Transparent dense sodium. Nature 2009, 458, 182–185. [CrossRef]

37. Liu, G.; Liu, H.; Feng, X.; Redfern, S.A.T. High-pressure phase transitions of nitroso N2Ti to a semiconductor with an unusual topological structure. Phys. Rev. B 2018, 97, 140104. [CrossRef]
38. Blöchl, P.E. Projector augmented-wave method. Phys. Rev. B 1994, 50, 17953. [CrossRef]
39. Kresse, G.G.; Furthmüller, J.J. Efficient Iterative Schemes for Ab Initio Total-Energy Calculations Using a Plane-Wave Basis Set. Phys. Rev. B 1996, 54, 11169. [CrossRef]
40. Perdew, J.P.; Burke, K.; Ernzerhof, M. Generalized Gradient Approximation Made Simple. Phys. Rev. Lett. 1996, 77, 3865. [CrossRef]
41. Perdew, J.P.; Zunger, A. Self-interaction correction density-functional approximations for many-electron systems. Phys. Rev. B 1981, 23, 5048–5079. [CrossRef]
42. Peters, K.; Wartanessian, S.; Sax, A.F.; Edgecombe, K.E.; Becke, A.D.; Flad, J.; Nesper, R.; Preuss, H.; Werner, H.J.; Knowles, P.J.; et al. Electron localization in solid-state structures of elements—Diamond structure. Angew. Chem. Int. Ed. Engl. 1992, 31, 187–188.
43. Beek, A.D.; Edgecombe, K.E. A simple measure of electron localization in atomic and molecular-systems. J. Chem. Phys. 1990, 92, 5397–5403.
44. Togo, A.; Tanaka, I. First principles phonon calculations in materials science. Scr. Mater. 2015, 108, 1–5. [CrossRef]
45. Chaput, L.; Togo, A.; Tanaka, I.; Hug, G. Phonon-phonon interactions in transition metals. Phys. Rev. B 2011, 84, 094302. [CrossRef]
46. Giannozzi, P.; Gironcoli, S.D.; Pavone, P.; Baroni, S. Ab initio calculation of phonon dispersions in semiconductors. Phys. Rev. B 1991, 43, 7231. [CrossRef]
47. Gonze, X.; Lee, C. Dynamical matrices, Born effective charges, dielectric permittivity tensors, and interatomic force constants from density-functional perturbation theory. Phys. Rev. B 1997, 55, 10355. [CrossRef]
48. Saal, J.E.; Kirklin, S.; Aykol, M.; Meredig, B.; Wolverton, C. Materials design and discovery with high-throughput density functional theory: The open quantum materials database (OQMD). JOM 2013, 65, 1501–1509. [CrossRef]
49. Kirklin, S.; Saal, J.E.; Meredig, B.; Thompson, A.; Doak, J.W.; Aykol, M.; Rühl, S.; Wolverton, C. The Open Quantum Materials Database (OQMD): Assessing the accuracy of DFT formation energies. NPJ Comput. Mater. 2015, 1, 1–15. [CrossRef]