Potential ultra-incompressible material ReN: first-principles prediction

Yanling Li$^{1,2,3}$, Zhi Zeng$^1$, Haiqing Lin$^3$

1.Key Laboratory of Materials Physics, Institute of Solid State Physics, Chinese Academy of Sciences, Hefei 230031, People’s Republic of China and Graduate School of the Chinese Academy of Sciences, Beijing 100049, People’s Republic of China
2.Department of physics, Xuzhou Normal University, Xuzhou 221116, People’s Republic of China
3.Department of Physics and Institute of Theoretical Physics, The Chinese University of Hong Kong, Shatin, Hong Kong, China.

(Dated: April 24, 2008)

Abstract

The structural, elastic and electronic properties of ReN are investigated by first-principles calculations based on density functional theory. Two competing structures, i.e. CsCl-like and NiAs-like structures, are found and the most stable structure, NiAs-like, has a hexagonal symmetry which belongs to space group $P6_3/mmc$ with $a=2.7472$ and $c=5.8180\ \AA$. ReN with hexagonal symmetry is a metal ultra-incompressible solid and has less elastic anisotropy. The ultra-incompressibility of ReN is attributed to its high valence electron density and strong covalence bondings. Calculations of density of states and charge density distribution, together with Mulliken atomic population analysis, show that the bondings of ReN should be a mixture of metallic, covalent, and ionic bondings. Our results indicate that ReN can be used as a potential ultra-incompressible conductor. In particular, we obtain a superconducting transition temperature $T_c\approx4.8$ K for ReN.

PACS numbers: 61.50.Ah, 71.15.Mb, 71.20.-b, 71.20.Be, 81.05.Bx

* Corresponding author. Email address: zzeng@theory.issp.ac.cn
I. INTRODUCTION

Transition metal nitrides are of intense interest for researchers. Not only do they offer the fundamental scientific challenge of finding methods to control, tune and enhance their peculiar physical properties, but they also have important technical applications such as cutting tools, oxidation-resisting materials, optical and magnetic apparatus. Transition metal nitrides possess particular mechanical, optical, electric, and magnetic properties, which attribute to their unusual electronic bonding (a mixture of covalent, metallic, and ionic bondings) and strong electron-phonon interaction. The higher valence electron density (VED) and the stronger hybridization between transition metal $d$ electrons and nonmetal $p$ electrons as well as less elastic anisotropy make some of them exhibit large incompressibility and high hardness, considered as powerful candidates of superhard materials.

At present, there are three kinds of transition metal nitrides confirmed: $X_3N_4$ ($X=$Hf, Zr), $YN_2$ ($Y=$Pt, Ir, Os), and $ZN$ ($Z=$Ti, Ta, Nb, Mo) Many works, including determination of the structure, discussion of elastic and electrical properties, have been carried out theoretically and experimentally. The interaction of experiment and first-principles calculation has become a powerful tool to predict, test and confirm the structure of the new materials. For example, jointing experiment and first-principles calculation, OsN$_2$, IrN$_2$, and $\delta$-MoN were identified as orthorhombic $Pnnm$, monoclinic $P2_1c$ and hexagonal $P6_3mc$ structures, respectively. The sites of nitrogen atoms in unit cell can be confirmed by theoretical calculation, which makes it possible to deeply study the mechanical, electronic and magnetic properties of transition metal nitrides. Haq and Meyer reported the superconducting and electrical properties of Re$_{1-x}$N$_x$ ($x=0.13$-$0.5$) by means of ion implantation experimental technique. The rhenium nitride with fcc structure was observed and the corresponding superconducting temperature $T_c$ value of 4.5-5.0 K was obtained. However, Isaev et al. pointed out that transitional metal mononitrides with ten and more valence electrons in the NaCl-type structure are dynamically unstable which has been verified in MoN and NbN. As such, ReN with face centered cubic structure maybe unstable mechanically. So the crystal structure of ReN remains an open question to date. Moreover, to the best of our knowledge, the mechanical property of ReN has not been reported.

In this paper, the structural, mechanical and electronic properties of ReN are investi-
gated by first-principles calculations. Because most of the transition-metal mono-nitrides are known to be generally based on cubic or hexagonal metal sublattice, and N atoms occupy octahedral or trigonal prismatic interstitial sites, therefore, all the possible cubic and hexagonal structures are chosen as candidate structures of ReN, including zinc blende (ZB) (space group \( F\overline{4}3m \)), rocksalt (NaCl) (space group \( Fm\overline{3}m \)), CsCl (space group \( Pm\overline{3}m \)), WC (space group \( P\overline{6}m2 \)), and NiAs types (space group \( P6_3/mmc \).\(^{19}\) Then incompressibility and elastic anisotropy are discussed. Further, the superconduction transition temperature \( T_c \) of ReN is estimated using the modified McMillan equation by Allen and Dynes.\(^{20}\) Finally, the electronic property of ReN is given by electron structure calculation and Mulliken atomic population analysis.

II. COMPUTATIONAL DETAILS

Our calculations on structural and electronic properties of ReN are based on the full-potential linearized augmented plane waves plus local orbitals method (FP-LAPW)\(^{21}\) as implemented in the Wien2k package to solve the scalar-relativistic Kohn-Sham equations.\(^{22}\) For the exchange correlation energy functional, the local density approximation (LDA) is employed. The muffin-tin radii are set to 1.9 and 1.60 bohr for Re and N, respectively. The maximum value \( l_{\text{max}} \) for the wave function expansion inside the atomic spheres is limited to 10. We expand the basis function up to \( R_{\text{MT}} K_{\text{max}} = 7.0 \) (\( K_{\text{max}} \) is the maximum modulus of the reciprocal lattice vector). Full relativistic approximation is used for the core electrons, and scalar relativistic approximation is used for the valence electrons of 5s5p4f5d6s for Re and of 2s2p for N. The self-consistent cycle is achieved by taking 1200 points in the first Brillouin zone. The convergence has been followed with respect to the energy and density.

The elastic constants of ReN are obtained within the framework of the finite strain technique by CASTEP code using first-principles plane-wave basis pseudopotential method (PW-PP) based on DFT.\(^{23}\) All the possible structures are also optimized by the BFGS algorithm\(^{24}\) which provides a fast way of finding the lowest energy structure and supports cell optimization in the CASTEP code. In the calculation, the interaction between the ions and the electrons is described by using Vanderbilt’s supersoft pseudopotential with the cutoff energy of 310 eV. In the geometrical optimization, all forces on atoms are converged to less than 0.002 eV/\( \text{Å} \), all the stress components are less than 0.02 GPa, and the tolerance
in self-consistent field (SCF) calculation is $5.0 \times 10^{-7}$ eV/atom. Relaxation of the internal
degrees of freedom is allowed at each unit cell compression or expansion. From the full elastic
contant tensor we determine the bulk modulus $B$ and the shear modulus $G$ according to
the Voigt-Reuss-Hill (VRH) approximation. The Young’s modulus, $E$, and Possion’s ratio,
$\nu$, can be calculated by the formulae $E = \frac{9BG}{3B+G}$, $\nu = \frac{3B-2G}{2(3B+G)}$.

III. RESULTS AND DISCUSSIONS

The equilibrium volume, bulk modulus and its pressure derivative are obtained by fitting
the total energy calculated at different volumes to the 3-rd order Birch-Murnaghan equation
of state. The equilibrium structural parameters, density, valence electron density, the total
energy, as well as the bulk modulus and its pressure derivative obtained from FP-LAPW
method are listed in Table I. The energy-volume curve is plotted in Fig. 1. ReN is more
energetically stable in the hexagonal structure under ambient pressure than cubic structure
and NiAs-ReN structure is most stable, as shown in Table I and Fig. 1. In NiAs-ReN (space
group $P\overline{6}_3/mmc$) the unit cell contains two chemical formula units (f.u.) in which two Re
atoms are at $2a$ (0, 0, 0) and two N atoms at $2c$ (1/3, 2/3, 1/4) sites. The equilibrium volumes per
formula unit (f.u.) are 23.5037 $\text{Å}^3$ for ZB-ReN, 19.5258 $\text{Å}^3$ for NaCl-ReN, 18.9065 $\text{Å}^3$ for
CsCl-ReN, 19.4775 $\text{Å}^3$ for WC-ReN, and 19.0162 $\text{Å}^3$ for NiAs-ReN, which are higher than
that of Re metal (14.7173 $\text{Å}^3$) due to the adding of N atoms. We note that the expansion
of lattice when incorporating the N in the pure Re is not high enough to compensate for
the decrease for the interatomic distance between the first neighbors. The nearest-neighbor
distance $d$ between atoms in ReN is much less than that of Re (which is about 2.74 Å),
which means that ReN maybe possess the much higher bulk modulus than pure Re metal
(discussed later). The densities of ReN are 14.1476, 17.0299, 17.5877, 17.0721, and 17.4862
$\text{g/cm}^3$, for ZB-ReN, NaCl-ReN, CsCl-ReN, WC-ReN, and NiAs-ReN, respectively.

The valence electron shell of Re is $5d^66s^2$, and that of N is $2s^2p^3$ so the total valence
electron number is 12 per ReN molecule. The calculated VEDs are 0.5106 electrons/$\text{Å}^3$
for ZB-ReN, 0.6146 electrons/$\text{Å}^3$ for NaCl-ReN, 0.6347 electrons/$\text{Å}^3$ for CsCl-ReN, 0.6162
electrons/$\text{Å}^3$ for WC structure, and 0.6310 electrons/$\text{Å}^3$ for NiAs-ReN. It is worthy to
note that all VEDs for these three structures are higher than that of Re metal (0.4761
electrons/$\text{Å}^3$) and are compared with 0.70 electrons/$\text{Å}^3$ for diamond. Generally, the
higher VED, the stronger the incompressibility. In addition, from Table I, it is clear that the bulk modulus of ReN is larger than that (360 GPa)\textsuperscript{28} of Re metal except for ZB-ReN (unstable mechanically). Thus, we conclude that the ReN is less compressible than the pure Re. It is delighted that the estimated bulk modulus of ReN with NiAs, CsCl, and WC structures is even comparable to that of diamond\textsuperscript{30} which means that the ReN with these structures has a stronger incompressibility, indicating that ReN can be a candidate of superhard material.

In order to get more accurate elastic constants of ReN using PW-PP scheme, all considered structures are optimized firstly\textsuperscript{31}. The calculated elastic constants are presented in Table II. For a stable hexagonal structure, the five independent elastic constants $c_{ij}$ ($c_{11}, c_{33}, c_{44}, c_{12}$ and $c_{13}$) should satisfy the well known Born-Huang criteria for stability:\textsuperscript{32}

\[ c_{12} > 0, c_{33} > 0, c_{11} > c_{12}, c_{44} > 0, (c_{11} + c_{12})c_{33} > 2c_{13}^2; \]

while for cubic crystal, the three independent elastic constants $c_{ij}$ ($c_{11}, c_{12}$ and $c_{44}$) satisfy inequalities:\textsuperscript{32}

\[ c_{44} > 0, c_{11} > |c_{12}|, c_{11} + 2c_{12} > 0. \]

Clearly, our calculated elastic constants $c_{ij}$ for both cubic CsCl-ReN and the hexagonal NiAs-ReN satisfy the Born-Huang stability criteria, suggesting that they are mechanically stable. Cubic ZB-ReN and NaCl types are unstable mechanically because of their negative $c_{44}$. Our results stand by for Isaev’s viewpoint of which the transition metal mononitrides with ten and more valence electrons in the NaCl-type structure are unstable mechanically. WC-ReN type is also unstable mechanically due to the very small $c_{44}$ value (near zero). In the following, only CsCl and NiAs types of ReN are discussed.

From the elastic constants calculated above, bulk modulus $B$, shear modulus $G$, Young’s modulus $E$, and Possion’s ratio $\nu$ are obtained and listed in Table II, which are important in order to understand the elastic properties of ReN. The bulk modulus of ReN calculated by using elastic constants agrees well with the one obtained through the fit to the 3rd order Birch-Murnaghan EOS, which shows that the discussion-above on compressibility of ReN is reasonable. To further discuss the incompressibility of ReN, the evolution of the volume compressions as a function of pressure are plotted in Fig. 2. For comparison, the volume compression of diamond is given simultaneously. It is evident that ReN with NiAs structure
is slight higher incompressible than diamond, while ReN with CsCl structure has slightly less incompressible than diamond in the entire pressure range (Fig. 2(b)).

To explain the directional dependence of compression, fraction axis compression as a function of pressure for diamond and two structures of ReN are given in Fig. 3. Compression of the axes presents interesting anisotropy. For hexagonal NiAl-ReN, the c axis is more incompressible than the a axis. The incompressibility along a-axis is slightly less than that of diamond, while c axis is even more incompressible than the analogous axis of diamond. While for cubic CsCl-ReN, it is slightly lower incompressible than diamond (Fig. 2 and Fig. 3). Therefore, we can claim that ReN is an ultra-incompressible solid. The shear moduli obtained are 248 GPa for CsCl-ReN and 237 GPa for NiAs-ReN, and corresponding G/B values are 0.588 and 0.526. The Possion’s ratio is 0.25 and 0.28 for CsCl and NiAs types, respectively, which indicates that ReN has central interatomic forces and is relatively stable against shear. The high G/B ratio or, equivalently, the low Poisson’s ratio also implies a high value degree of covalency.

It is well known that the elastic anisotropy of crystals has significant application in engineering science since it is highly correlated with both the hardness of materials and the possibility to induce microcracks in the materials. Hence it is important to calculate elastic anisotropy in order to understand the properties and improve the durability of materials. The anisotropy factor for cubic CsCl-ReN, \( A = \frac{2c_{44} + c_{12}}{c_{11}} = 0.45 \), shows that cubic CsCl-ReN is elastic anisotropy. The anisotropy of linear compression along the a axis and c axis with respect to the b axis can be evaluated by means of two parameters: \( A_{B_a} \) and \( A_{B_c} \), where a value of 1 indicates compression isotropy and any departure from one corresponds to a degree of compression anisotropy. For low symmetry crystal, the percentage of anisotropy in compressibility and shear can be derived from two expressions, bulk modulus anisotropic factor \( A_B \) and shear anisotropy factor \( A_G \), respectively. The calculated linear compression parameters \( A_{B_a}, A_{B_c} \) and two other anisotropy factors \( A_B \) and \( A_G \) are listed in Table III. NiAs-ReN is almost isotropy in compressibility (0.317%) and has slightly shear anisotropy (\( A_G = 4.199\% \)). From Table III, one can see that cubic CsCl-ReN is compression isotropy, and hexagonal ReN’s c axis has much stronger incompressibility than that of a axis, which is in good agreement with fractional axis compression analysis mentioned above. The small elastic anisotropy of NiAs-ReN, including linearized compressibility and shear anisotropy, along with the ultra-high bulk modulus and the higher shear modulus (or \( c_{44} \)), indicates
that NiAs-ReN can be as a good candidate of superhard material. Comparing $c_{44}$ with shear modulus for hexagonal NiAs-ReN, we find that they are almost the same, imaging that NiAs-ReN hardness can be given a consistent estimation by the viewpoints on hardness from Teter and Jhi et al. Here, using the correlation between shear modulus and Vickers harness given by Teter, the estimated Vickers hardness of ReN are 33.6 GPa for CsCl-ReN and 32.1 GPa for NiAs-ReN, and 36.2 GPa for MoN-ReN. All the hardness of ReN presented here are comparable to that of B$_6$O (35±5GPa) and that of TiB$_2$ (33±2GPa).

The Debye temperature correlates with many physical properties of solids, such as elastic constants, specific heat, melting temperature and superconduction transition temperature. Since the vibrational excitations mainly arise from acoustic vibrations at low temperature, the Debye temperature obtained from elastic constants is the same as that determined from specific heat measurements. The Debye temperature can be derived by bulk modulus, shear modulus and density $\rho$. The calculated Debye temperature $\Theta_D$s are as high as 968 K for CsCl-ReN and 950 K for NiAs-ReN, which indicates that ReN maybe a superconductor. So, we further estimate the superconducting transition temperature of ReN with NiAs structure using the modified McMillan equation, where the electron-phonon coupling constant $\lambda$ is calculated by density-functional perturbation theory by means of the QUANTUM ESPRESSO package. The calculated $\lambda$ is 1.67 and the estimated superconducting transition temperature $T_c$ is about 4.8 K for the screened Coulomb pseudopotential $\mu^*$ equal to 0.1, which agrees well with available experimental result.

To understand the correlation between the electronic properties and the mechanical properties, we present density of states (DOS) and the electron density distribution of ReN in the equilibrium geometry. Electronic structure properties play an important role in material physical properties. The total density of states (DOS) and partial DOS of two phases of ReN are shown in Fig. 4 and Fig. 5. The obtained $N(E_F)$ and the linear specific heat coefficient $\gamma$ are given in Table I. The finite value $N(E_F)$ shows that ReN is a metal. For two phases, the electrons from Re-$d$ and the N-$p$ states both contribute to the DOS near the Fermi level. The peak emerging in the lower energy region of the DOS curve mainly originates from the localized $s$ states of N. The energy region just above Fermi level is dominated by unoccupied Re-$d$ states. The DOS of Re-$d$ and N-$p$ are energetically degenerate from the bottom of the valence band to the top of conduction band, indicating the possibility of covalent bonding between Re and N atoms. The covalent characteristic between Re and N atoms can be
confirmed by the charge density distribution. The charge density distribution in (110) plane for CsCl-ReN and (1120) plane for NiAs-ReN are shown in Fig. 6 (a) and (b), respectively. It is clearly seen that a strong directional bonding exists between Re and N in the ReN, which contributes to high bulk modulus $B$, namely, strong incompressibility of ReN. Additionally, the Mulliken atomic population analysis is carried out by using CASTEP code. The obtained total charge transfer from Re to N in CsCl-ReN (NiAs-ReN) is 0.55 (0.62), implying that the chemical bondings between Re and N have some characteristics of ionicity. Thus our results demonstrate that the bondings should be a mixture of covalent, mental, and ionic attribution in ReN.

IV. CONCLUSION

The structural, elastic, and electronic properties of different structures for ReN are investigated based on first-principles calculation under the framework of density functional theory within local density approximation. Two competing structures, i.e., CsCl-ReN and NiAs-ReN, are found. High valence electron density, strong incompressibility and low elastic anisotropy indicate that ReN is an ultra-incompressible superhard solid. Electron structure calculation shows that ReN presents an obvious metal feature. In particular, we obtain a superconducting transition temperature $T_c \approx 4.8$ K for hexagonal ReN. The strong hybridization between metal $d$-electron and nonmetal $p$-electron are observed, indicating that there is a strong covalent bonding between Re and N. From Mulliken atomic population analysis along with discussion of mechanical and electronic properties, it can be concluded that the bondings in ReN should be a mixing of metal, ionic and covalent characteristics. Our results indicate that ReN can be used as a potential ultra-incompressible conductor. We hope this work can stimulate the experimental research for ReN.

This work was supported by the National Science Foundation of China under Grant Nos 10504036 and 90503005, the special Funds for Major State Basic Research Project of China(973) under grant no. 2005CB623603, Knowledge Innovation Program of Chinese Academy of Sciences, and Director Grants of CASHIPS. Part of the calculations were per-
formed in the Shanghai Supercomputer Center.

1 E. Horvath-Bordon, R. Riedel, A. Zerr, P. F. McMillan, G. Aufermann, Y. Prots, W. Bronger, R. Kniep, and P. Kroll, Chem. Soc. Rev. 35, 987 (2006).
2 P. F. McMillan, Nat. Mater. 1, 19 (2002)
3 A. Zerr, G. Miche, and R. Riedel, Nat. Mater. 2, 185 (2003).
4 J. C. Crowhurst, A. F. Goncharov, B. Sadigh, C. L. Evans, P. G. Morrall, J. L. Ferreira, and A. G. Nelson, Science 311, 1275 (2006).
5 A. F. Young, C. Sanloup, E. Gregoryanz, S. Scandolo, R. J. Hemley, and H. K. Mao, Phys. Rev. Lett. 96, 155501 (2006).
6 E. Soignard, O. Shebanova, and P. F. McMillan, Phys. Rev. B 75, 014104 (2007).
7 C. L. Bull, P. F. McMillan, E. Soignard, and K. Leinenweber, J. Solid State Chem. 177, 1488 (2004).
8 R. B. Kaner, J. J. Gilman and S. H. Tolbert. Science 308, 1268 (2005).
9 M. Mattesini, R. Ahuja, and B. Johansson, Phys. Rev. B 68, 184108 (2003).
10 A. F. Young, J. A. Montoya, C. Sanloup, M. Lazzeri, E. Gregoryanz, and S. Scandolo, Phys. Rev. B 73, 153102 (2006).
11 Z. W. Chen, X. J. Guo, Z. Y. Liu, M. Z. Ma, Q. Jing, G. Li, X. Y. Zhang, L. X. Li, Q. Wang, Y. J. Tian, and R. P. Liu, Phys. Rev. B 75, 054103 (2007).
12 R. Yu, Q. Zhan, and L-C. De Jonghe, Angew. Chem. Int. Ed. 46, 1136 (2007).
13 Z. Wu, X. Hao, X. Liu, and J. Meng, Phys. Rev. B 75, 054115 (2007).
14 J. A. Montoya, C. Sanloup, E. Gregoryanz, and S. Scandolo, Appl. Phys. Lett. 90, 011909 (2007).
15 C. Z. Fan, S. Y. Zeng, L. X. Li, Z. J. Zhan, R. P. Liu, W. K. Wang, P. Zhang, and Y. G. Yao, Phys. Rev. B 74, 125118 (2006).
16 M. B. Kanoun, S. Goumri-said, and M. Jaouen, Phys. Rev. B 76, 134109 (2007).
17 A. ul. Haq and O. Meyer, J. Low Temp. Phys. 50, 123 (1983).
18 E. I. Isaev, S. I. Simak, I. A. Abrikosov, R. Ahuja, Yu. Kh. Vekilov, M. I. Katsnelson, A. I. Lechtenstein, and B. Johansson, J. Appl. Phys. 101, 123519 (2007).
19 The δ-MoN (space group $P6_3/mc$) type is also considered in our research. It is found that $δ$-
MoN type is also stable mechanically and has a strong incompressibility (bulk modulus $B$, 451 GPa; shear modulus $G$, 267 GPa). Symmetry analysis show that the MoN-ReN structure is a slight distortion of the supercell (2×2×1) of NiAs-ReN structure. The unit cell ($a=5.4981$ and $c=5.8095$ Å) of MoN-ReN contains eight f.u. with eight Re atoms occupying $2a$ (0, 0, 0.5481) and $6c$ (0.4996, 0.5004, 0.5472) sites and eight N atoms holding $2b$ ($\frac{1}{4}$, $\frac{2}{4}$, 0.7994) and $6c$ (0.1667, 0.8333, 0.2986) sites. The NiAs-ReN and MoN-ReN have the very similar structural parameters, which result in the almost same total energy per f.u. (differing only by 5 meV) and the similar mechanical and electronic properties. So, the results of $\delta$-MoN type is not given in the text.

20 P. B. Allen and R. C. Dynes, Phys. Rev. 12, 905 (1975).
21 E. Sjöstedt, L. Nordström, and D. J. Singh, Solid State Commun. 114, 15 (2000); G. K. H. Madsen, P. Blaha, K. Schwarz, E. Sjöstedt, and L. Nordström, Phys. Rev. B 64, 195134 (2001).
22 P. Blaha, K. Schwarz, G. Madsen, D. Kvasnicka, and J. Luitz, computer code Wien2k, an augmented plane wave plus local orbitals program for calculating crystal properties, Karlheinz Schwarz, Technische Universität Wien, Austria, 2001.
23 M. D. Segall, P. J. D. Lindan, M. J. Probert, C. J. Pickard, P. J. Hasnip, S. J. Clark, M. C. Payne, J. Phys.: Cond. Matt. 14, 2717 (2002).
24 B. G. Pfrommer, M. Cote, S. G. Louie, and M. L. Cohen, J. Comput. Phys. 131, 133 (1997).
25 R. Hill, Proc. Phys. Soc. London 65, 349 (1952).
26 F. Birch, Phys. Rev. 71, 809 (1947); J. -P. Poirier, Introduction to the physics of the Earth’s Interior, Cambridge University Press, Cambridge, 2000.
27 G. S-Neumann, L. Stixrude, and R. E. Cohen, Phys. Rev. B 60, 791 (1999).
28 H. Chung, A. B. Weinberger, J. B. Levine, A. Kavner, J. Yang, S. H. Tolbert, and R. B. Kaner, Science 316, 436 (2007).
29 J. J. Gilman, R. W. Cumberland, and R. B. Kaner, Int. J. Refrac. Mat & Hard Mat. 24, 1-5 (2006).
30 F. Occelli, D. L. Farber, and R. L. Toullec, Nat. Mater. 2, 151 (2003); J. C. Zheng, Phys. Rev. B 72, 052105 (2005).
31 All calculated parameters using PW-PP method agree well with those given by using FP-LAPW method within 1.0%, showing that the PW-PP method can be used to calculate the elastic properties of ReN.
32 M. Born and K. Huang, Dynamical Theory of Crystal Lattices (Clarebdom, Oxford, 1956).
33 P. Ravindran, L. Fast, P. A. Korzhavyi, B. Johansson, J. Wills, and O. Eriksson, J. Appl. Phys. 84, 4891 (1998).

34 D. M. Teter, MRS. Bull. 23, 22 (1998).

35 S-H. Jhi, J. Ihm, S. G. Louie, and M. L. Cohen, Nature 399, 132 (1999).

36 O. L. Anderson, J. Phys. Chem. Solids 24, 909 (1963).

37 P. Giannozzi et al., http://www.quantum-espresso.org
FIGURE CAPTIONS

Fig.1: (Color online) The total energy per ReN molecule as a function of volume (EOS).

Fig.2: (Color online) Volume as a function of pressure with respect to equilibrium volume. $V_0$ is the equilibrium volume.

Fig.3: (Color online) Fractional axis compression as a functional of pressure. $a_0$, $b_0$, and $c_0$ are lattice parameters of equilibrium volume at zero pressure.

Fig.4: (Color online) Partial and total DOS for the CsCl phase of ReN obtained from FP-LAPW calculations. Vertical dotted lines indicate the Fermi level.

Fig.5: (Color online) Partial and total DOS for the NiAs phase of ReN obtained from FP-LAPW calculations. Vertical dotted lines indicate the Fermi level.

Fig.6: The valence electron density contour for ReN obtained from FP-LAPW. Charge density is in an increment of 0.01 $e$/a.u.$^3$ from 0.01 $e$/a.u.$^3$ to 0.12 $e$/a.u.$^3$. (a) (110) plane for CsCl-ReN; (b) (12\(\bar{2}0\)) plane for NiAs-ReN.
TABLE CAPTIONS

TABLE I: Equilibrium lattice parameters, $V_0$ (Å$^3$), $a$ (Å), $c$ (Å), $c/a$, the shortest Re-N distance $d$, density $\rho$ (g/cm$^3$), valence electron densities $\rho_e$ (electrons/Å$^3$), bulk modulus $B_0$ and its pressure derivative $B_0'$, relative total energy $E_{tot}$ (eV), DOS at Fermi level $N(E_F)$ (States/eV/cell), and the linear specific heat coefficient $\gamma$ (mJ/mol.cell.K$^2$). $V_0$ and $E_{tot}$ are of per chemical f.u.

TABLE II: Zero-pressure elastic constants $c_{ij}$ (GPa), the isotropic bulk modulus $B$ (GPa), shear modulus $G$ (GPa), Young’s modulus $E$ (GPa), Possion’s ratio $\nu$, average elastic wave velocity $v_m$ (m/s), and Debye temperature $\Theta_D$.

TABLE III: The bulk modulus along the crystallographic axes $a$, $b$, and $c$ ($B_a$, $B_b$, and $B_c$) for ReN. Percent elastic anisotropy for shear and bulk moduli $A_G$ (in %), $A_B$ (in %) and compressibility anisotropy factors $A_{B_a}$ and $A_{B_c}$ for ReN obtained from LDA calculations. Here, $A_{B_a} = \frac{B_a}{B_b}$, $A_{B_c} = \frac{B_c}{B_b}$. 
|                | Li et al.                |
|----------------|-------------------------|
|                | ZB-ReN  NaCl-ReN  CsCl-ReN  WC-ReN  NiAs-ReN |
| $V_0$          | 23.5037  19.5258  18.9065  19.4775  19.0162 |
| $a$            | 4.5468  4.2743  2.6640  2.7476  2.7472 |
| $c$            | 2.9786  5.8180 |
| $d$            | 1.9688  2.1371  2.3073  2.1759  2.1523 |
| $\rho$         | 14.1476  17.0299  17.5877  17.0721  17.4860 |
| $\rho_e$       | 0.5106  0.6146  0.6347  0.6161  0.6310 |
| $B_0$          | 340  406  412  433  453 |
| $B_0'$         | 4.241  4.729  4.542  4.319  4.203 |
| $E_{tot}$      | 0.444  1.328  1.623  0.610  0.0 |
| $N(E_F)$       | -  -  1.220  -  1.674 |
| $\gamma$       | -  -  2.88  -  3.95 |
### TABLE II: Li et al.

|                | $c_{11}$ | $c_{33}$ | $c_{44}$ | $c_{12}$ | $c_{13}$ | $B$  | $G$  | $E$  | $\nu$ | $\Theta_D$ |
|----------------|----------|----------|----------|----------|----------|------|------|------|-------|------------|
| ZB-ReN         | 297      | -715     | 356      | 336      | -255     | -1025| -    | -    | -     | -          |
| NaCl-ReN       | 456      | -334     | 372      | 400      | -27      | -83  | -   | -    | -     | -          |
| CsCl-ReN       | 1015     | 164      | 124      | 421      | 248      | 622  | 0.25| 968  |       |            |
| WC-ReN         | 640      | 654      | 0.55     | 240      | 368      | 429  | 53  | 152  | -     | -          |
| NiAs-ReN       | 712      | 897      | 236      | 314      | 278      | 450  | 237 | 604  | 0.28  | 950        |

### TABLE III: Li et al.

|                | $B_a$ | $B_b$ | $B_c$ | $A_{B_a}$ | $A_{B_c}$ | $A_B$ | $A_G$ |
|----------------|-------|-------|-------|-----------|-----------|-------|-------|
| CsCl-ReN       | 1264  | 1     | 0     | 11.55     |           |       |       |
| NiAs-ReN       | 1237  | 1627  | 1     | 1.3155    | 0.317     | 4.199 |       |
FIG. 1: Li et al.
FIG. 2: Li et al.
FIG. 3: Li et al.
FIG. 4: Li et al.
FIG. 5: Li et al.
FIG. 6: Li et al.