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First-principles investigations of the physical properties of RCd (R=Ce, La, Pr, Nd)

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ABSTRACT

The crystal structural, electronic, elastic and the thermodynamic properties of RCd are investigated by using the first-principles plane-wave pseudopotential density function theory within the generalized gradient approximation (GGA). The calculated equilibrium lattice parameters for RCd are in good agreement with the available experimental data. Furthermore, the optical properties, namely the dielectric function, refractive index and electron energy loss are reported for radiation up to 30 eV. Finally, the elastic properties, the bulk modulus and the Debye temperature of RCd are given for reference.

1. Introduction

Many rare-earth equiatomic compounds crystallize RM (R=rare earth, M=metal) have been extensively investigated in the past [1,2], taking advantage of their versatility with respect to changes in the magnetic moment. Kitai et al. measured the magnetic property of PrCd single crystal in the temperature range from 4.2 K to 300 K [3]. Fujii et al. studied the magnetization and susceptibility of NdCd and CeCd [4]. Although some physical constants such as electrical resistivity, thermoelectric power, thermal conductivity and magnetic properties [5–7] have been reported in many papers, the electronic structures, optical properties, elastic properties and the Debye temperature are still unclear, further investigations is necessary to clarify their physical properties. Base on above, in this work, we calculated the crystal structural, electronic, elastic properties and the Debye temperature of RCd by using the first-principle method in order to reveal a complete understanding of the basically physical properties.

The present work is organized as follow: In the next Section, we describe briefly the method of calculation Section 3 contain our results and discussion, involving structural properties, electronic structures, optical properties, elastic properties and the Debye temperature for the RCd. Finally, the paper ends with a conclusion where we summarize our main findings are given in Section 4.

2. Calculation methods

In this paper, first-principles calculations are performed within CASTEP [8] based on the density function theory (DFT). The exchange and correlation functional was treated by the generalized gradient approximation (GGA) with the PBEsol [9], respectively. Cutoff energy of plane-wave is 500 eV and a $7\times7\times7$ Monkhorst-Pack (MP) k-point mesh has been employed in this study to ensure well convergence between the computed structures and energies. The structural parameters optimization were calculated using the Brodyden–Fletcher–Goldfarb–Shanno (BFGS) method, with the threshold for converged structures: the maximum energy change of per atom is 5×10^{-6} eV/

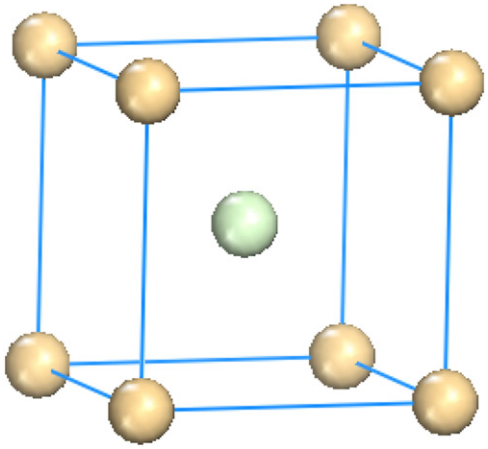

Fig. 1. Crystal structure of RCd (M=Ce, La, Pr, Nd) compounds.

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atom, the maximum Hellmann–Feynman force of per atom is 1×10^{-2} eV/Å, the maximum stress within 2×10^{-2} GPa and the maximum displacement of atom is 5×10^{-4} Å during the geometry optimization. The electronic configurations were following: $4d^{10}5s^2$ for Cd; $4f^15s^25p^65d^16s^2$ for Ce; $5s^25p^65d^16s^2$ for La; $4f^35s^25p^66s^2$ for Pr and $4f^45s^25p^66s^2$ for Nd. Interaction between the ionic cores and valence electrons was described by the ultrasoft pseudopotentials.

Table 1
Calculated structure parameters of RCd in our work compared with the experimental data.

Compound	Method		a (Å)	V(Å^3)	ρ (g/cm^3)
CeCd	PBEsol	Cal.	3.83873	56.5668	7.41312
		Exp.	3.85500[a]	57.2893	7.31963
LaCd	PBEsol	Cal.	3.90425	59.5132	7.01221
		Exp.	3.91000[b]	597765	6.98132
PrCd	PBEsol	Cal.	3.79767	54.7709	7.68007
		Exp.	3.82700[c]	56.0500	7.50482
NdCd	PBEsol	Cal.	3.78042	54.0280	7.88808
		Exp.	3.81900[d]	55.6992	7.65141

[a] Reference[11].
[b] Reference[11].
[c] Reference[11].
[d] Reference[11].

The optical properties of crystal are studied by the frequency-dependent dielectric function $\varepsilon(\omega)=\varepsilon'(\omega)+i\varepsilon''(\omega)$ that is mainly connected with the electronic structures. The imaginary part $\varepsilon''(\omega)$ of the dielectric function is calculated from the momentum matrix elements between the occupied and unoccupied electronic states and given by [10]

$$\varepsilon''(\omega)=\frac{2e^2\pi}{\Omega\varepsilon_0}\sum_{k,v,c}|<\psi_k^c|\hat{u}\times r|\psi_k^v>|^2\delta(E_k^c-E_k^v-E) \quad (1)$$

where u is the unite vector defining the polarization of the incident electromagnetic wave, ω is the light frequency of the incoming photons, e is the electronic charge,ψ_k^c and $\psi_k^v$are the conduction and valence band wave functions at k, respectively. Since the dielectric constant describes a causal response, the real and imaginary parts are linked by a Kramers–Kronig transform. All other optical constants such as the refractive index, absorption coefficient and energy-loss spectrum can be computed from the values of $\varepsilon(\omega)$. The calculated

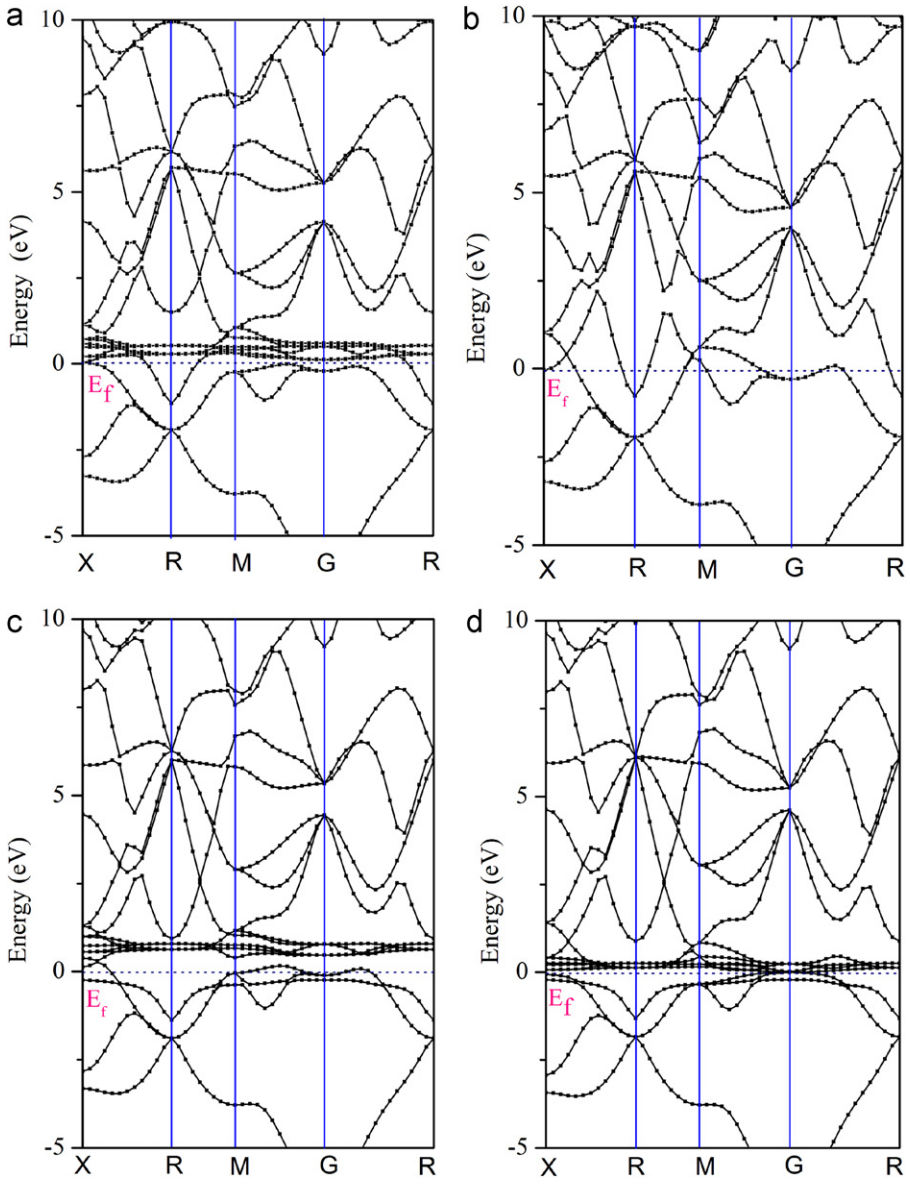

Fig. 2. Band structure of RCd compounds: (a) CeCd (b) LaCd (c) PrCd (d) NdCd.