Development of Transferable Materials Information and Knowledge Base for Computational Materials Science

Project Representative

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The multi-industry CAMP program on the Earth Simulator (ES) is focused on dealing with various kinds of nanostructure materials of which calculated results are to be used as integrated information of comprehensive skills and knowledge base on computational materials science. Discussions in the FY2005 are, mainly, focused on two typical methods to utilize calculated results to overcome multi-scale problems. We have developed two programs by which we can obtain information on the electronic structures of the atom in Coulomb potential field in materials and the interatomic potential energy from cluster calculations applying the modified Mobius transformation based on the number theory. Our approach is applicable to other extended systems.

Keywords: pseudo-atom, inverse problem, pair potential, nanostructure materials, knowledge base

1. Overview of the Project

One of the most important problems in the computational materials science is the multi-scale one; the first principles calculation can not always provide efficient information for the classical molecular dynamical potential parameters to overcome the threshold between the nano-scale and meso-scale systems. The goal of our project is to create the integrated knowledge base by exploiting calculated nanostructure material databases. We have developed two codes in the ES during FY2003–2005. One is for the non-periodic nanostructure system for molecules and clusters by the standard linear combination of atomic orbitals method using the norm-conserving pseudopotential (LCAO-PS). The other one is for the periodic system, CAMP-Atami, which focuses on electronic structures for not only ground states but excited ones by solving the time-dependent Schrödinger equation based on the standard density functional theory (TDDFT). The characteristic feature in our approach is that the Schrödinger equation is solved on a real space in both codes. In FY2004, we have developed an interface between LCAO-PS and CAMP-Atami code. In this FY2005, we developed two schemes to obtain physical information from calculated databases; the oxygen charge density and potential field and interatomic pair potential from the nano-metal cluster calculations.

2. Atom in materials

We summarize our method on the multi-center numerical integration scheme by dividing any physical quantity into

each atomic site with a localized fuzzy cell type weight function as follows.

$$F(\vec{r}) = \sum_{\alpha=1}^{N} F_\alpha(\vec{r}_\alpha) \quad F_\alpha(\vec{r}_\alpha) = w_\alpha(\vec{r}_\alpha) F(\vec{r})$$

where $\quad \vec{r}_\alpha \equiv \vec{r} - \vec{R}_a \quad \sum_{\alpha=1}^{N} \omega_\alpha(\vec{r}_\alpha) = 1 \quad ^\forall \vec{r}_\alpha$

$$I = \sum_{\alpha=1}^{N} I_\alpha \quad I_\alpha = \int F_\alpha(\vec{r}_\alpha) d\vec{r}_\alpha$$

The numerical integration points are given by one-dimensional radial part and two-dimensional spherical grids; typically 50 times 200 at each atomic site to obtain 6-digit accuracy. The parallelization of computing whole physical quantities is performed by atomic site using MPI. Each physical quantities requires us $O(N^2)$ calculation after determining the Coulomb potential field. It is the most important problem to calculate the accurate Coulomb potential and energy in the DFT. The key point in our treatment is that the Coulomb potential is given by just superimposing each contribution from each atomic site, which is completely parallelized by using MPI, i.e. $O(1)$; it takes typically 20 seconds irrespective to the number of atomic sites.

$$v_c(\vec{r}) = \sum_{\alpha=1}^{N} v_c(\vec{r}_\alpha) \Leftarrow MPI$$

$v_c(\vec{r}_\alpha) = v_c(r_\alpha) y_{\ell m}(\hat{r}_\alpha) \quad y_{\ell m}(\hat{r}_\alpha) \, spherical \, harmonic \, function$

$$v_c(r_\alpha) = \sum_{\ell m}^{\ell_{max}} \frac{4\pi}{2\ell+1} \left[\int_0^{r_\alpha} \frac{r^\ell \, \rho_\alpha^{\ell m}(r)}{r_\alpha^{\ell+1}} \, dr + \int_r^\infty \frac{r_\alpha^\ell \, \rho_\alpha^{\ell m}(r)}{r^{\ell+1}} \, dr \right]$$

$$\rho(\vec{r}) = \sum_{\alpha=1}^{N} \rho_\alpha^{\ell m}(r_\alpha) y_{lm}(\hat{r}_\alpha)$$

Our present code had been modified so as to be able to pick up a kind of pseudo-atom for an arbitral number of charge by controlling the shape of ω. We can utilize them as the initial charge density and potential field to construct materials. Figure 1 shows spherically averaged radial distribution of O^{2-} charge density difference from the free atom in various oxides. O^{2-} does not change significantly in various systems. Figure 2 is an example of non-spherical charge density and potential field. Figures 3 and 4 represent the atomic energy levels of O^{2-} in typical oxides. In Al_2O_3, it is shown that O^{2-} is more stable than O^{1-}. Energy levels of the atom in oxides agree very well with the bulk density of states.
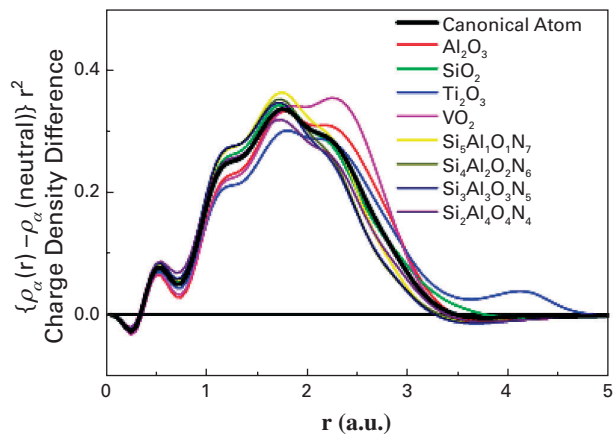

Fig. 1 Spherically averaged radial charge distribution of O^{2-} charge density difference from the free atom in various oxides. Canonical means the averaged one.
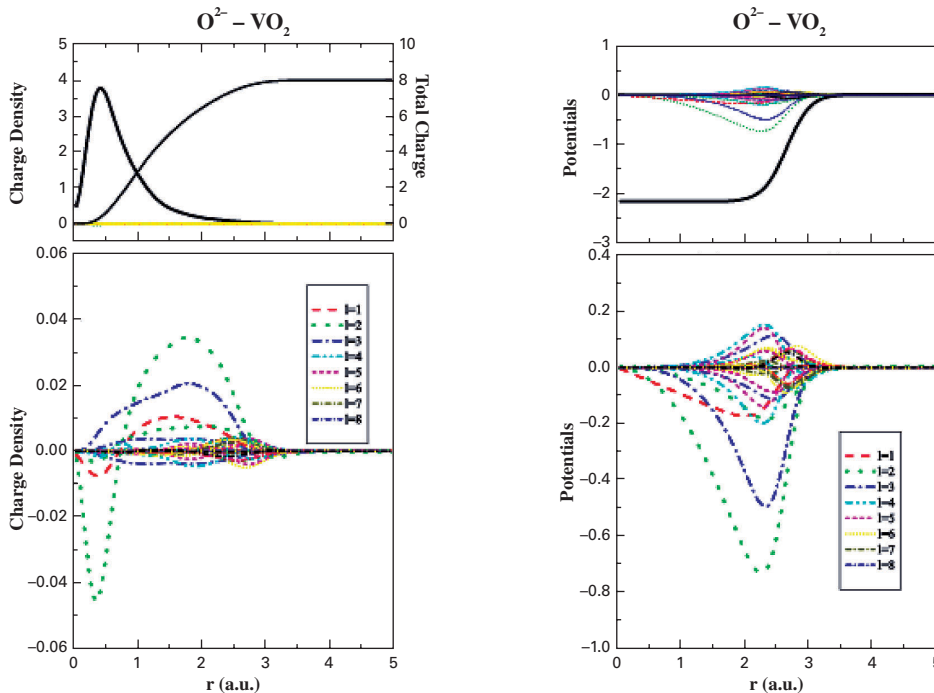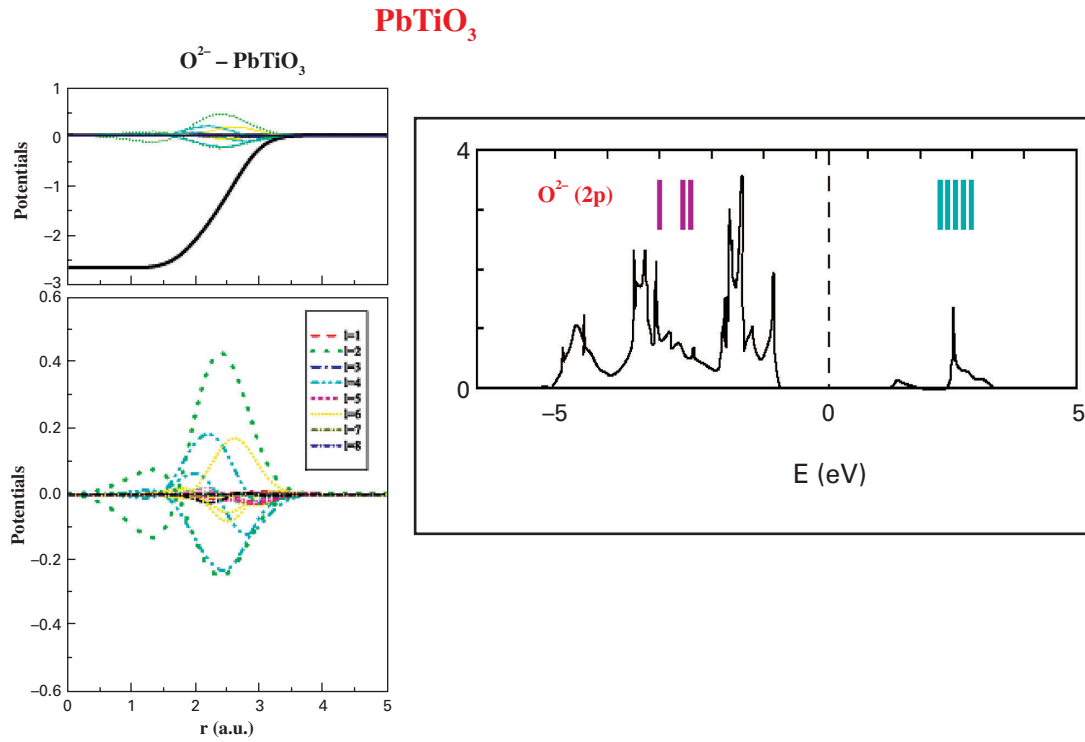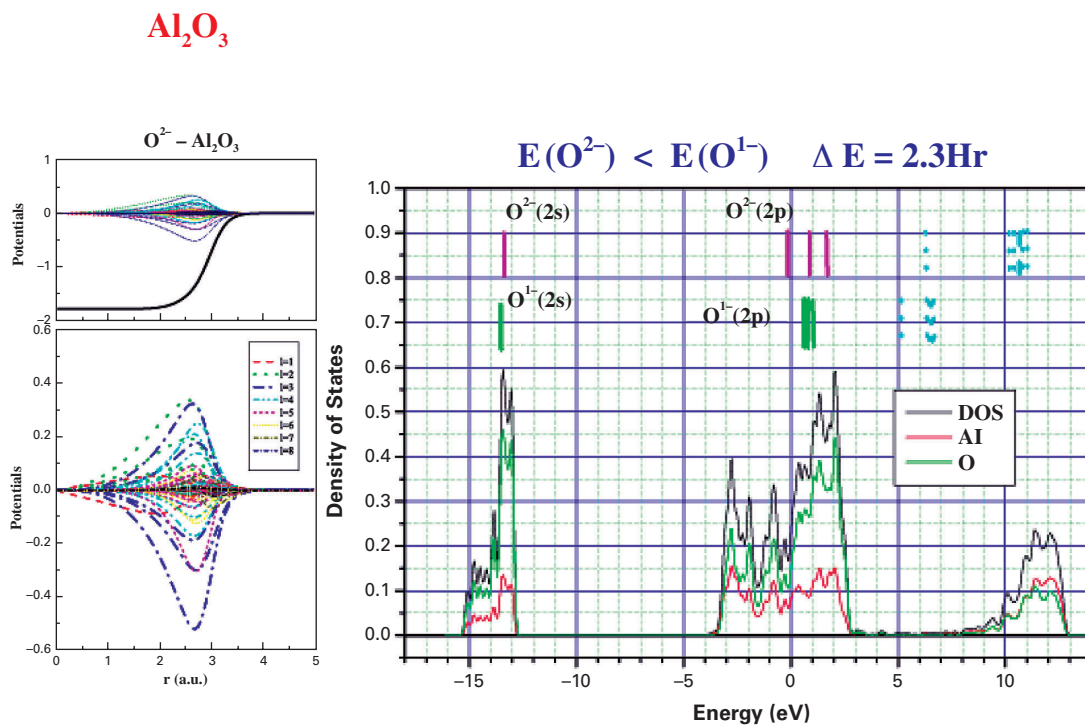

Fig. 2 Non-spherical charge density and potential field for O^{2-} in VO_2. ℓ is the degree of spherical harmonics.

PbTiO₃

O²⁻ – PbTiO₃

Fig. 3 Potential field and energy levels of O^{2-} in PbTiO₃.

Al₂O₃

O²⁻ – Al₂O₃

$$E(O^{2-}) < E(O^{1-}) \quad \Delta E = 2.3 Hr$$

Fig. 4 Potential field and energy levels of O^{1-} and O^{2-} in Al₂O₃. Total energy of O^{2-} ion is more stable than O^{1-}.

3. Inverse problem

The inverse problem is one of the most important ones in terms of the modeling for the first principles calculation. Applying the well known Mobius transformation, Chen[1] developed a 3-dimensional inverse transformation scheme, modified Mobius transformation, for the system of a case of the periodic lattice. We applied it to the cluster system.

$$E_b(r) = \frac{1}{2}\sum_{\alpha \neq 0}\Phi\left(|\vec{R_\alpha}|\right) = \sum_{n=1}\omega(n)\Phi(\sqrt{n}r)$$

$$\Phi(r) = \sum_{n=1}\mu(n)E_b(\sqrt{n}r)$$

$$\sum_{n|k}\omega(n)\mu(k|n) = \delta_{1k}$$

$E_b(r)$ is the binding energy of the cluster determined by the first principles calculation and Φ is the pair potential. $\vec{R_\alpha}$ represents the lattice position. $\omega(n)$ is the number of equivalent sites at the distance r. $\mu(n)$ is the modified Mobius function which is determined by the semi-group property with respect to the lattice periodicity related with the multiplication of $\sqrt{n}$. Figure 5 shows examples of pair potential energies by this scheme.

4. Summary

We have been developing parallel codes for dealing with transferable knowledge base during these three years. The efficient computation by the ES provided us to not only produce direct simulation data but create and utilize knowledge base obtained from the self-consistent results. Our treatment will be efficient to develop further materials design in any situation.

References

[1] N.X.Chen, Phys.Rev.Lett.64, 1193 (1990)
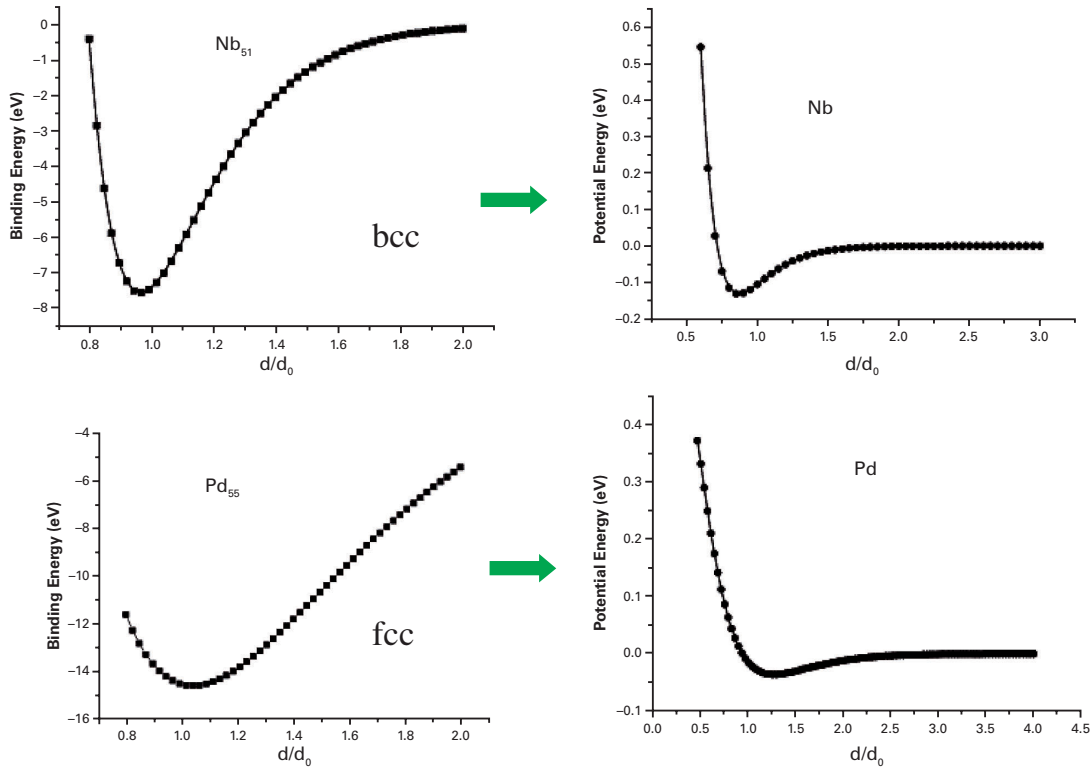[2] Q.Xie and Nan-Xian Chen, Phys.Rev.B 51, 15856 (1995).

Fig. 5 Interatiomic pair potential determined from nano-metal clusters, Nb_{51}(bcc) and Pd_{55}(fcc), using the modified Mobius transformation scheme.

計算材料科学のための物質情報構築法の開発

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　2003 年度から3年計画で始まったCAMP-ES プロジェクトは、最終年をむかえた。本プロジェクトは、非周期系と周期系の2種類のシステムが取り扱える2つのプログラムの開発によって、データ共有と知識ベース化による計算の効率化向上 を目的とした異業種企業間共同研究プロジェクト である。過去2年間で開発したプログラムは、分子・クラスターなどの非周期系のためのLCAO-PSクラスターコードと、結晶系の計算コードCAMP-Atamiである。本プロジェクトにおける物質系シミュレーションは、単 なる計算機実験だけではなく、よりインテリジェントな擬似原子を計算結果から抽出し、物質内の原子がどのような環境にあるかを調べたり、マルチスケール問題に対応 できるようエネルギー計算から原子間ポテンシャルを求めたりして、次への認識のステップへの道筋をつけることである。物質系の知識ベースの例として酸素イオンがどのような環境下にあるかという事例とナノクラスター計算から変形メビウス変換を用いて原子間ポテンシャルを求めた結果を示す。

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