Project Title: Development of new long-range corrected density functional theory and its applications

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1. Background and purpose of the project, relationship of the project with other projects

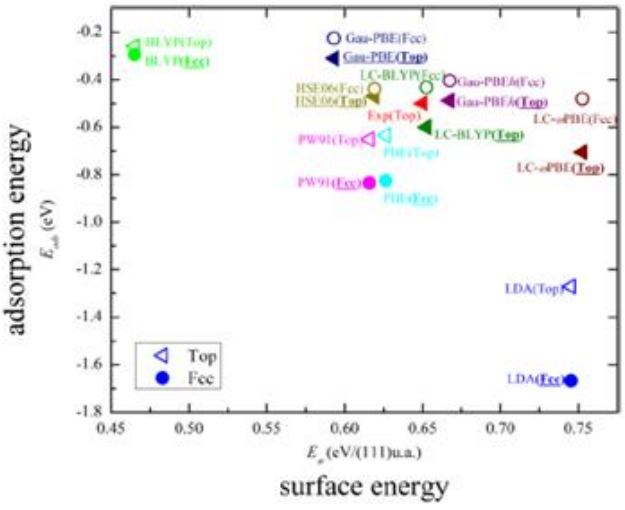
The prediction of adsorption energy using theoretical methods is valuable and useful for developing new materials for green energy. However currently there are no efficient DFT method able to reproduce both the experimental adsorption energies between CO molecule and metal surfaces. The PBE functional underestimates surface energy of Pt(111) and Rh(111) and overestimates adsorption energy of CO molecule to Pt(111) and Rh(111) surfaces. Meanwhile, BLYP functional underestimates surface energy even though it provides the adsorption energy in relatively high accuracy. The results calculated using the HSE screened hybrid functional show the inclusion of the short-range HF exchange integral leads to little improvement. Another problem of conventional DFT functionals in the calculations of adsorption energies is that they cannot predict the experimental adsorption site preferences. Recently, we developed the linear-scaled Long-range corrected (LC-) DFT [LC-DFT(2Gau)], which enables LC-DFT functional to be applied to solid-state material calculations. In this project, we applied LC-DFT(2Gau) method to the surface and adsorption energy calculations of Cu metal surface and CO molecule.

2. Specific usage status of the system and calculation method

In this project, we used 100% of gwacsg (65,508 hour) and more than 43% of bwmpc (601,129 hour) for this project and other researches which will be submitted to publicaions.

3. Result

We applied LC-DFT(2Gau) functional to the adsorption energies between CO molecule and Cu(111) surface and the surface energies of Cu(111), with the results showing that LC-DFT (especially, LC-BLYP) reproduces well both adsorption and surface energies, and predicts correctly the experimental adsorption site preferences shown in the figure. Importantly, this research demonstrates that the LC-DFT functional yields accurate energy preferences between top and fcc site, even though other DFT functionals shows indistinguishable energy gaps between top and fcc sites or contrary preferences.



4. Conclusion

In this project, we applied the linearly-scaled LC-DFT to solid state system and showed possible applicability of LC-DFT to solid state calculations.

5. Schedule and prospect for the future

We will extend the application of LC-DFT to Pt and Rh metal surface for the calculations of adsorption

energy and will see effectiveness of long-rang corrections. Moreover, we will hopefully apply the linearly-scaled LC-DFT to the optical band-gap calculations of solid state using time-dependent (TD) scheme. We expect that TD-LC-DFT will provide highly improved predictions for molecule-adsorbed semi-conductor systems. The success of such development would enable applicability to surface chemistry by providing cost-effective theoretical method for high accuracy band-gap predictions of surface science and solar energy conversion technology for the development of efficient materials for DSSC.

Usage Report for Fiscal Year 2017

Fiscal Year 2017 List of Publications Resulting from the Use of the supercomputer

[Oral presentation at an international symposium]

1. "Development of DFT functional applicable to large molecular and periodic systems" J.-W. Song The 120th General Meeting of the Korean Chemical Society (Area: Recent Progress in Electronic Structure Theory) PHYS1-4 (2017.10.19.), Kwangju, Korea. [Invited]
2. "Theory: A New partitioning scheme to model dispersion coefficients. Application: Study of thermochromic properties of PDAs via TD-DFT" U. V. Ucak and J.-W. Song The 12th Daegu-Saga-Soochow University International Joint Symposium, L-3 (2017.11.20.), Gyeongsan-si, Korea. [Invited]
3. "Theoretical investigations on Metal Ion Selectivity of Thiophene Derivative Compounds" Jin jae Lee, Seung Hyun Chang, and Jong-Won Song The 12th Daegu-Saga-Soochow University International Joint Symposium, P-50 (2017.11.20.), Gyeongsan-si, Korea.
4. "Inside or Outside?: Quantum Chemical Studies on Intermolecular Binding Energy between Carbon Nano-tube and Aromatic Molecules" Dae-Hwan Ahn and J.-W. Song, The 12th Daegu-Saga-Soochow University International Joint Symposium, P-49 (2017.11.20.), Gyeongsan-si, Korea.