Assignment 1

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December 2020

1 Question 1

1.1 Pseudopotentials for quantum Monte Carlo studies of transition metal oxides

Strengths

• Psuedopotential removes the high energy core electrons and thus simplifies the problem.In this paper highly accurate Psuedopotential are generated using DFT approximations.

• QMC with the generated Psuedopotential could calculate first through fourth ionization potential of transition metal(M).

• QMC with the generated Psuedopotential calculated binding curve of M-O dimer. From that binding energy and bond length are found.

• Optimized Psuedopotential give accurate result to the study of bulk transition metals.

Weakness

• For CrO calucalated data is highly deviated from experimental data.

• For weakly bound Cuo and ZnO largest deviation from RCCSD(T) study occurs.

[1]

1.2 Binding energies of trions and biexcitons in two-dimensional semiconductors from diffusion quantum Monte Carlo calculations

Strengths

•Gives statistically exact diffusion monte carlo binding energy data for Mott-Wannier models of trions, excitons and biexcitons in the 2D semiconductors.

•Provide contact pair densities to allow description of contact (exchange) interactions between charge carriers using first-order perturbation theory.

•Data indicate that the binding energy of a trion is generally larger than that of a biexciton in 2D semiconductors.

Weakness

• For the biexciton, there is a major disagreement between theory and experiment.

[2]

References

[1] J. T. Krogel, J. A. Santana, and F. A. Reboredo, "Pseudopotentials for quantum monte carlo studies of transition metal oxides," *Phys. Rev. B*, vol. 93, p. 075143, Feb 2016. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevB.93.075143

[2] M. Szyniszewski, E. Mostaani, N. D. Drummond, and V. I. Fal'ko, "Binding energies of trions and biexcitons in two-dimensional semiconductors from diffusion quantum monte carlo calculations," *Phys. Rev. B*, vol. 95, p. 081301, Feb 2017. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevB.95.081301

2 Question 2

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2.1 Home page

My Home page.

2.2 Projects Page

My Project Page