Usage Report for Fiscal Year 2019

Project Title:

Emergent magnetism by correlation effects in carbon-based materials (CARBOMAG)

Name:

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

In this project, we plan to use quantum Monte Carlo (QMC) methods, instead of density functional theory, to describe the electronic and magnetic states developing in carbon-based materials with peculiar structural settings, such as graphene nanoribbons and graphene vacancies and impurities. QMC is one of the most promising theories to study strong correlation effects from first principles, because electron correlation is explicitly taken into account via a correlated wave function. This wave function can be shaped to be as close as possible to the ground and excited states of the system.

2. Specific usage status of the system and calculation method

The project is in its production phase, with large scale jobs ready to be submitted, after a period of testing, and parameters set up for the system, such as the basis set, k-point and system size convergence study.

3. Result

We determined the optimal basis set for carbon nanoribbon calculations, and the optimal supercell sizes to be simulated in order to reduce the finite size errors. Calculations in the paramagnetic, ferromagnetic, superconducting and spin fluctuating phases are ongoing.

4. Conclusion

We devised a scheme to perform finite size scaling in an efficient way for quantum Monte Carlo calculations of graphene nanoribbons. We applied the geminal embedding method to derive an optimal contracted basis set, which will allow us to carry out QMC wave function optimizations in extended periodic calculations.

5. Schedule and prospect for the future

In the remaining months, we are going to perform simulations of the most relevant phases of graphene nanoribbons to unveil the energetics of this system, provide benchmarks, and understand its viability for technologically relevant applications.

6. If no job was executed, specify the reason.

Fiscal Year 2019 List of Publications Resulting from the Use of the supercomputer

[Paper accepted by a journal]

[Conference Proceedings]

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[Oral presentation]

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[Poster presentation]

Tomonori Shirakawa, “Local multiplet structure and emergence of spin in graphene with a single vacancy”, International Conference on Strongly Correlated Electron Systems 2019 (SCES2019), Sep. 20, 2019, Okayama.

[Others (Book, Press release, etc.)]

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