

Adiabatic-Connection Interpolation Model with Broader Applicability

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ABSTRACT

In the Adiabatic Connection Integrand Interpolation (ACII) method, the electronic correlation is obtained by interpolating between the weak-interaction limit, which includes both the exact-exchange and the second-order Görling-Levy (GL) perturbation term, and the strong-interaction limit. In the last years, several ACII functionals have been proposed for different topics[1], yet an accurate ACII model with broader applicability is still missing. Here, we propose an ACII approach, named genISI2[2] with a superior performance with respect to other ACII functionals, for both three-dimensional (3D) and two-dimensional 2D extended systems, for the Hook's atom and for molecular systems, as shown in Fig. 1.

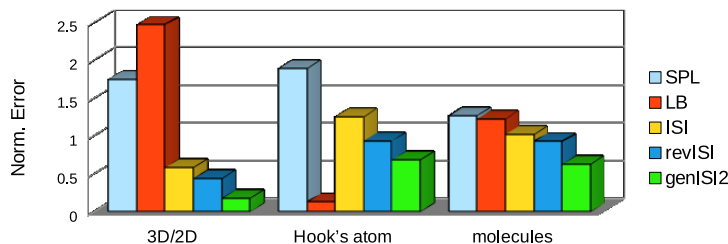


Figure 1: Normalized errors for several tests for different ACII functionals.

References

- [1] Constantin, L. A.; Jana, S.; Śmiga, S.; Della Sala, F., "Adiabatic connection interaction strength interpolation method made accurate for the uniform electron gas", *J. Chem. Phys.* **2023**, *159*, 244111
- [2] Constantin, L. A.; Śmiga, S.; Della Sala, F., "Towards adiabatic-connection interpolation model with broader applicability", **2024**, <http://arxiv.org/abs/2403.07391>.