Dopyqo:
Many-body analysis on top of DFT calculations

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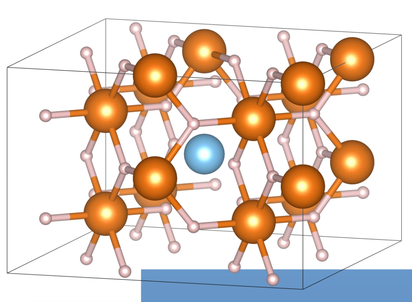
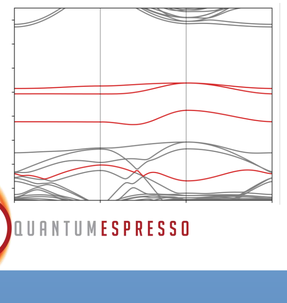
pip install dopyqo

DLR-WF/Dopyqo

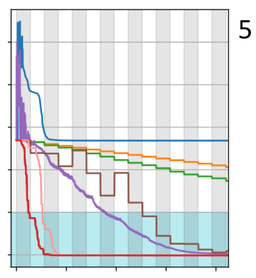
Introduction

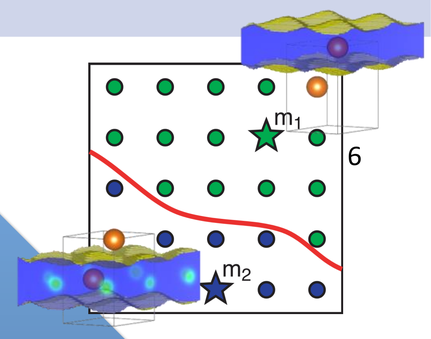
Quantum chemistry and condensed matter physics are among the most promising applications of quantum computers. Further, estimating properties of materials is crucial to evaluate their industrial applications. Dopyqo[1] bridges the gap between DFT and many-body simulations of periodic systems by building many-body Hamiltonians and solving them using classical and quantum algorithms. The Hamiltonians are computed from Kohn-Sham orbitals obtained from a prior Quantum ESPRESSO[2] DFT calculation. We present the usefulness of Dopyqo by calculating partial atomic charges for strongly correlated systems and comparing them to DFT and DFT+U.





$$\hat{H}^{(\mathbf{k})}_{\text{elec}} = \sum_{tu} h^{(\mathbf{k})}_{tu} \hat{a}^\dagger_t \hat{a}_u \quad \text{(1-electron terms)}$$
$$+ \frac{1}{2} \sum_{tuvw} h^{(\mathbf{k})}_{tuvw} \hat{a}^\dagger_t \hat{a}^\dagger_u \hat{a}_v \hat{a}_w \quad \text{(2-electron terms)}$$
$$+ E_{\text{n-n}} \quad \text{(nuclear interaction)}$$
$$+ E_{\text{e-self}} \quad \text{(electron self-energy)}$$





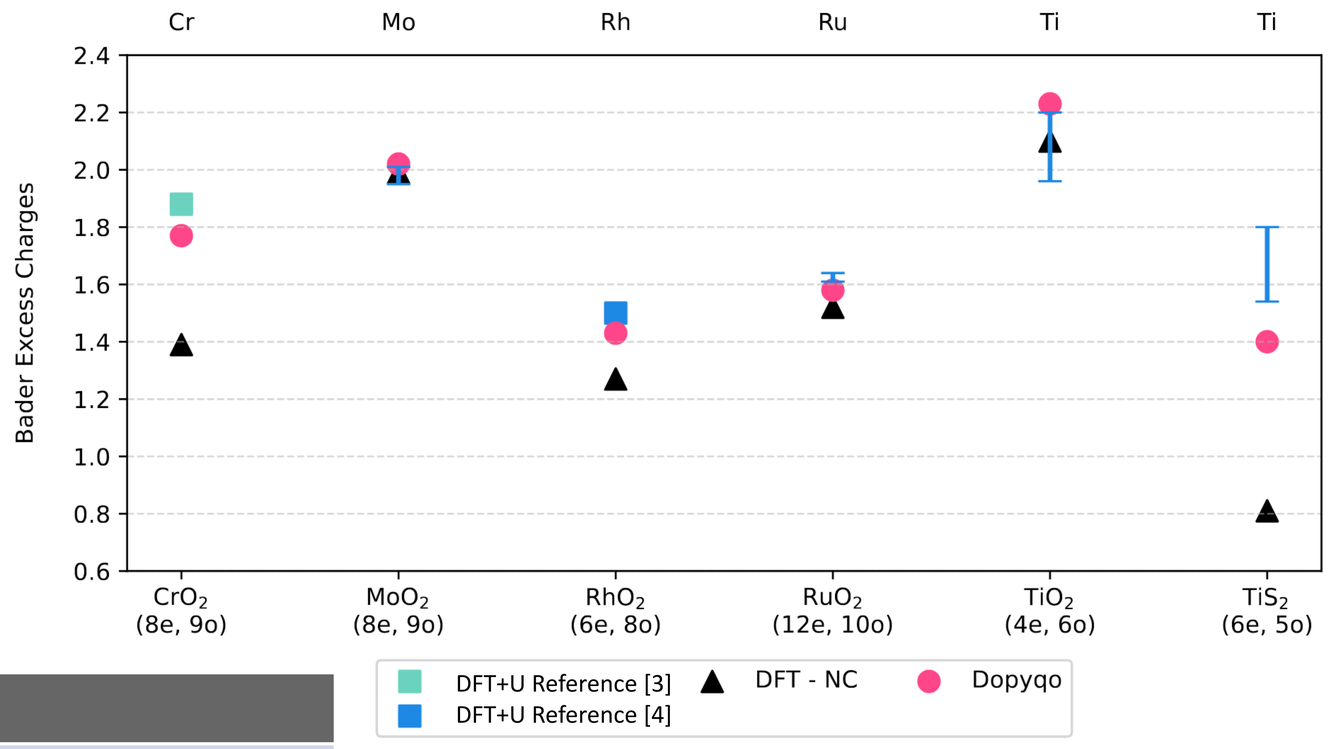
Material → DFT Simulation → Many-body Hamiltonian → Ground state → Properties

Use-case example: Bader charges

Bader charges[5] are solely based on the charge density which is a central quantity in DFT and can be calculated from a many-body wavefunction. First, Bader regions B_I are computed. Integrating the charge density within one Bader region yields the Bader charge Q_I of that region: $Q_I = \int_{B_I} \rho(\boldsymbol{r})\, \mathrm{d}^3\boldsymbol{r}$. If a Bader region encapsules one nucleus the Bader charge of that region is assigned to the atom of that nucleus. We compute the density as $\rho(\boldsymbol{r}) = \sum_t f_t |\psi_t(\boldsymbol{r})|^2$ with occupations f_t^{VQE} from VQE: $f_t^{\text{VQE}} = \langle \Psi_{VQE} | \hat{n}_t | \Psi_{VQE} \rangle$.

Summary

- Exact electronic structure calculations of periodic systems
- Starting from DFT simulations
  - Kohn-Sham and Wannier orbitals
- Solve active space with FCI, VQE, ADAPT-VQE
- Improved Bader charges relative to DFT towards DFT+U reference
- Other features in preparation: Bulk modulus, geometry optimization



Sources

[1] Schultheis et al., 2025, arXiv
[2] Giannozzi et al., 2009, J. Phys.: Condens. Matter
[3] Lu et al., 2018, Phys. Rev. B
[4] Choudhuri et al., 2020, J. Chem. Theory Comput.
[5] Jäger et al., 2025, arXiv
[6] Tang et al., 2009, J. Phys.: Condens. Matter

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