Contribution ID: **53**

Type: **Contributed Oral**

Subtraction of orbital self-interaction from the Kohn-Sham equations

Tuesday 2 December 2025 17:45 (15 minutes)

The effective design of new materials for sustainable energy conversion can be facilitated by the accurate prediction of electronic properties with moderate computational complexity and cost. The self-interaction error (SIE) of Kohn-Sham density functional theory (KS-DFT) is a non-physical, non-linear dependence of an orbital's energy on its own fractional occupation [Dabo et al., Phys. Rev. B, 82:115121, 2010]. The generalized Koopmans condition (GKC) ensures an atomic orbital's eigenenergy is invariant with its own fractional occupation, and is free of self-interaction. The constrained search of the Levy spin-density-functional theory yields orbital densities and delivers the ground-state energy in accordance with the Hohenberg-Kohn theorems. In this work, the electron density of the Kohn-Sham equations is thereby constrained to be orbital-density dependent, with a total energy functional linear with respect to variation of its orbital densities. That is, the KS multiplicative effective potential $v_{\mathrm{s}}[n]$ for an orbital $\varphi_i[n]$ is constrained to a functional $v_{\mathrm{eff}}[n - n_i]$. The result complies with the generalized Koopmans condition (GKC). Preliminary calculations show fundamental band gaps with an accuracy comparable to the G_0W_0 approximation of many-body perturbation theory (MBPT), with a level of complexity comparable to KS-DFT. In practice, software codes can be combined to remove SIE and to model composite material properties. With the subtraction of non-physical electron self-interaction from the Kohn-Sham equations, GKC-DFT can possibly improve computational efficiency, reduce the complexity of highly accurate DFT simulations, and facilitate the development of new applications.

Author: INGALL, John (The University of Newcastle, Australia)

Co-author: Prof. PAGE, Alister (The University of Newcastle, Australia)

Presenter: INGALL, John (The University of Newcastle, Australia)

Session Classification: Condensed Matter & Materials

Track Classification: Topical Groups: Condensed Matter & Materials