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Black-box, accurate, and efficient prediction of band structures with Koopmans functionals — •Edward Linscott[1], Nicola Colonna[1], Junfeng Qiao[2], and Nicola Marzari[1,2] — [1]Paul Scherrer Institut, Villigen, Switzerland — [2]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Over the past fifteen years we have developed Koopmans functionals, a computationally efficient approach for predicting spectral properties in a functional framework [1]. These orbital-density-dependent functionals impose a generalized piecewise linearity condition that ensures that orbital energies match the corresponding electron removal/addition total energy differences (in contrast to semi-local DFT, where a mismatch between the two lies at the heart of the band gap problem and the unreliability of Kohn-Sham band structures more generally). Koopmans functionals prove to be very powerful, yielding band structures and molecular orbital energies and with comparable accuracy to self-consistent GW approaches but at greatly reduced computational cost and complexity [2]. This talk will cover the theory of Koopmans functionals and how recent developments – namely, the development of automated workflows via the `koopmans` code [3] and projectability-based Wannierization [4] – have brought us one step closer to black-box prediction of accurate band structures.

[1] Dabo et al., PRB 82 (2010), Borghi et al., PRB 90 (2014); [2] Nguyen et al., PRX 8 (2018), Colonna et al., JCTC 15 (2019); [3] koopmans-functionals.org, Linscott et al., JCTC 19 (2023); [4] Qiao et al., npj Comput. Mater. 9, 206 & 208 (2023)

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