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Theoretical spectroscopy of organic semiconductors: challenges and progress

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The combination of density functional theory (DFT) with powerful spectroscopic tools, e.g., photoemission spectroscopy or absorption spectroscopy, is an important approach to elucidating the electronic structure of materials. In recent years, it has become a particularly popular tool for studying organic semiconductors and their interfaces with inorganic substrates - topics of great importance in organic electronics. Here I review our recent progress in understanding the strengths, limitations, and true predictive power of such analyses. In particular, the consequences of self-interaction and derivative discontinuity errors and the importance of long-range exchange and correlation are analyzed. I then show how this allows for the a priori selection and incorporation of the correct "physical ingredients" into (typically) orbital-dependent functionals. Finally, via judicious comparison with a variety of pertinent experimental results on prototypical organic electronic molecules and structures, I show that this approach results in quantitatively accurate calculations of properties often considered to be "too difficult for standard DFT."