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Charged excitations in extended nanostructures from Koopmans-compliant functionals NICOLAS POILVERT, ISMAILA DABO, Department of Materials Science and Engineering, The Pennsylvania State University — Koopmans-compliant (K) functionals aim to restore the piecewise linearity of approximate density-functional theory (DFT) functionals, generalizing ideas first introduced in the case of DFT+U functionals, but not restricted to predefined atomic orbitals. K functionals enable one to recover meaningful energy levels, which can thus be interpreted as charged excitation energies. Although it has been shown that K calculations yield energy levels and cross sections in excellent agreement with photoelectron spectroscopies, applications to crystalline materials have been lacking. Here, we report on recent progress in describing the band structures of periodic systems within K approximations. Our approach proceeds by analyzing the response of the electron density upon charged excitation in the limit of increasingly large systems. This analysis underscores important differences between conventional DFT approximations and their K counterparts, and enables us to generalize K functionals to extended systems. Validation of this approach is provided by the accurate description of sp^2-bonded carbon nanostructures. In the process, we highlight the performance of common DFT approximate functionals in capturing charged excitations in materials, provided that electronic localization is enforced

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