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A Self-consistent Mixing Parameter Scheme for Hybrid Functionals Applied to Periodic Systems[1] JONATHAN SKONE, MARCO GOVONI, Department of Chemistry, University of California, Davis, GIULIA GALLI, Institute for Molecular Engineering, Univesrity of Chicago — We present a self-consistent scheme for determining the optimal fraction of exact exchange (α) for hybrid functionals applied to condensed phase systems. It has been previously shown that the optimal mixing parameter is related to the inverse of the dielectric constant in solids, which in turn is related to the statically screened exchange term in the electronic self-energy within the GW approximation. We use this relationship to evaluate α self-consistently so as to obtain a mixing-parameter that is independent of the (arbitrary) choice of the initial fraction of exact-exchange. Our self-consistent scheme (sc-EXX) does not rely on any empirical parameters and is straightforward to apply to semiconducting and insulating, periodic systems. We show that for a variety of solids the sc-EXX scheme yields macroscopic dielectric constants in excellent agreement with experiment and provides considerable improvement in quasi-particle gaps over other non-empirical hybrid functionals with fixed exact exchange (e.g. PBE0). Furthermore, this approach provides an affordable way of capturing the static screening effects in a self-consistent manner, thus providing a superior starting point for GW calculations that include full dynamical screening.

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