SEMINARIO
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Screened hybrid functionals for solid-state physics and chemistry

This presentation will address our current efforts to develop more accurate exchange-correlation functionals for density functional theory. One of the functionals to be discussed is a screened hybrid known as HSE [1], which is particularly well suited for calculations of solids because it is much faster than regular hybrids and can also be used in metals. HSE yields an important improvement in band gap predictions [2] compared to LDA, GGAs, and meta-GGAs. We will also present applications to transition metal oxides, silicon phase transitions and defects [3], and other problems where electron localization seems to play a crucial role [4]. Preliminary results regarding the development of a promising new local hybrid will also be discussed.


