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New hybrid functionals for ab-initio calculations of properties of solids

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This presentation will address our current efforts to develop more accurate exchange-correlation functionals for Density Functional Theory. The functional to be discussed is a screened Coulomb potential exchange hybrid called **HSE** [1], which is particularly suited for calculations in solids because it is much faster than regular hybrids and can also be used in metals and systems with negligble band gaps. **HSE** yields an important improvement in band gap estimates [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].

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