北京大学量子材料科学中心

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Seminar

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地点 北京大学物理楼，西 会议室

Abstract

Density functional theory (DFT) is a powerful tool both in the fundamental understanding of materials and in the design of functional properties at the level of quantum mechanics. However, its accuracy is strongly limited by the adopted approximations of electron exchange correlation. Hybrid functional by including a fraction of exact exchange (EXX) overcomes the limitations of (semi)local approximations of DFT. Moreover,EXX is a basic ingredient in modern approaches to compute excitation properties, such as GW. So far, however, the demandingcomputational cost has limited the applications of EXX in plane wave calculations for extended systems. We show that this difficulty can be overcome by performing a unitary transformation from Bloch to maximally localized Wannier functions in combination with an efficient technique to compute real space Coulomb integrals. The resulting scheme scales linearly with system size and, when used in *ab initio* molecular dynamics simulations, requires only a modest increase in computational cost compared to standard DFT.

We validate the scheme by the accurately computed H-bond structures, the photoemission spectra, and the X-ray absorption spectra of H-bonded liquids, and the state-of-art theory of proton transfer though hydronium and hydroxide ions in liquid water solutions.