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Hybrid DFT orbitals as a means of reduction of fixed-node errors in diffusion Monte Carlo simulations JINDRICH KOLORENC, SHUMING HU, LUBOS MITAS, North Carolina State University — We explore possibilities to improve variational freedom of Slater-Jastrow trial wave function by using one-body orbitals from the hybrid density-functional theory (DFT) to construct its determinantal Slater part. Weight of the exact exchange term in the hybrid DFT functional serves as a variational parameter that is optimized with respect to the total energy calculated within the fixed-node diffusion Monte Carlo method. This approach is certainly less powerful than direct optimization of one-body orbitals within a basis-set expansion, but its modest computational requirements make it suitable for large-scale simulations of solids. Presented method will be illustrated on several materials with emphasis on transition-metal compounds. The weight of the exact exchange term optimized in this way can also serve as a guide for the hybrid DFT itself. For instance, it provides hints how the weight is changed/screened when a crystal is compressed.

Jindrich Kolorenc
North Carolina State University

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