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**Quantum Monte Carlo simulation of transition metal compounds employing the full Coulomb interaction** BRIGITTE SURER, PHILIPP WERNER, MATTHIAS TROYER, ETH Zurich, ANDREAS LAEUCHLI, MPI-PKS Dresden, EMANUEL GULL, Columbia, JAN KUNES, Augsburg, ALEXANDER LICHTENSTEIN, Hamburg — The recently developed Krylov implementation of the hybridization expansion impurity solver [arXiv:0908.0681] allows an efficient simulation of large multi-orbital models with full Coulomb interactions. In combination with density functional theory and dynamical mean field theory (DMFT) the method opens a way to investigate transition metal and actinide compounds from first principles. We will present applications of this algorithm to five-orbital models.

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