Abstract Submitted
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Obtaining model parameters for real materials from ab-initio calculations: Heisenberg exchange[1] DMITRY KOROTIN, Institute of Metal Physics, Yekaterinburg, VLADIMIR MAZURENKO, Ural Federal University, Yekaterinburg, VLADIMIR ANISIMOV, SERGEY STRELTSOV, Institute of Metal Physics, Yekaterinburg — An approach to compute exchange parameters of the Heisenberg model in plane-wave based methods is presented. This calculation scheme is based on the Green's function method and Wannier function projection technique. It was implemented in the framework of the pseudopotential method and tested on such materials as NiO, FeO, Li_2MnO_3, and $KCuF_3$. The obtained exchange constants are in a good agreement with both the total energy calculations and experimental estimations for NiO and $KCuF_3$. In the case of FeO our calculations explain the pressure dependence of the Néel temperature. Li_2MnO_3 turns out to be a Slater insulator with antiferromagnetic nearest neighbor exchange defined by the spin splitting. The proposed approach provides a unique way to analyze magnetic interactions, since it allows one to calculate orbital contributions to the total exchange coupling and study the mechanism of the exchange coupling.

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Dmitry Korotin
Institute of Metal Physics, Yekaterinburg

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