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Applying Density Functional Theory for Atomic Vacancies in Solids XIAOLAN ZHOU, Dept. of Physics, Tulane U., New Orleans, LA 70118, JOHN P. PERDEW, Dept. of Physics, Tulane U., New Orleans LA 70118 — We use a new generalized gradient approximation of density functional theory – PBEsol, a revised Perdew-Burke-Ernzerhof GGA, to calculate the vacancy formation energies and other properties of metals and semiconductors: Al, Pt, Pd, GaN [1], etc. By restoring the gradient expansion over a wide range of density gradients, PBEsol [2] yields excellent jellium exchange and correlation surface energies. We expect that this new functional will improve the description of vacancies in real materials, since the vacancy formation energy is essentially the work needed to create an interior surface.

[1] Thomas R.Mattsson and Ann E. Mattson. Phys. Rev. B **66**, 214410 (2002).
[2] John P. Perdew, Adrienn Ruzsinszky, Gabor I. Csonka, Oleg A. Vydrov, Gustavo E. Scuseria, Lucian A. Constantin, Xiaolan Zhou, and Kieron Burke, Restoring the density-gradient expansion for exchange in solids and surfaces, http://arxiv.org/abs/0711.0156

Adrienn Ruzsinszky
Dept. of Physics, Tulane U., New Orleans LA 70118

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