

PBEsol, a generalized gradient approximation for solids and their surfaces

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Successful modern generalized gradient approximations (GGA's) are biased toward atomic energies. Restoration of the first-principles gradient expansion for the exchange energy over a wide range of density gradients eliminates this bias. With many collaborators, I introduce PBEsol, a revised Perdew-Burke-Ernzerhof GGA that improves equilibrium properties of densely-packed solids and their surfaces.