Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Registry-dependent interlayer potential for graphitic systems ALEKSEY KOLMOGOROV, Duke University, VINCENT CRESPI, Pennsylvania State University — Standard applications of density functional theory (the local density approximation (LDA) and the generalized gradient approximation (GGA)) without nonlocal corrections do not adequately describe the exfoliation energy of graphite. The GGA, in particular, does not show any binding at physically meaningful interlayer distances. However, the *variation* in the energy under interlayer shifts, defined predominantly by the overlap of π orbitals, is nearly identical in the two approximations and appears to be much more sound than previously suspected. We combine these results with experimental information on the exfoliation energy to create an improved registry-dependent classical potential for the interlayer interaction in graphitic structures.

Aleksey Kolmogorov
Duke University

Date submitted: 23 Nov 2005 Electronic form version 1.4