Abstract Submitted
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A Quantum Monte Carlo investigation of dispersion interactions in graphite[1] LEONARDO SPANU, UC Davis Chemistry Department, Davis CA, GIULIA GALLI, UC Davis, Chemistry Department, Davis CA, SANDRO SORELLA, SISSA-ISAS, Trieste Italy — We present a series of Quantum Monte Carlo (QMC) calculations of graphite, aimed at describing on the same footing the strong C-C covalent bonds and the weaker interlayer interactions. In particular, we carried out calculations of binding energies, bond lengths and compressibility by using the Variational Monte Carlo and Lattice Regularized Diffusion Monte Carlo techniques [1]. We use as a variational ansatz the Jastrow Antisymmetrical Wave function, including a pairing determinant and a Jastrow correlation factor [2]. Our results allow for a detailed analysis of dispersion forces between graphite layers, including their behavior at long distances, and yield a quantitative estimate of the layer binding energy.

[1] Casula M. et al. Phys. Rev. Lett. 95 100201 (2005)
[2] Casula M. et al. J. Chem. Phys. 119, 6500 (2003)

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