Abstract Submitted
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The nature and strength of inter-layer binding in graphite[1] LEONARDO SPANU, Chemistry Department, UC Davis, Davis CA, SANDRO SORELLA, International School for Advanced Studies SISSA-ISAS and Democritos Trieste, Italy, GIULIA GALLI, Chemistry Department and Physics Department UC Davis, Davis CA — We compute the interlayer bonding properties of graphite using an ab initio many-body theory. We carry out variational and diffusion quantum Monte Carlo calculations and find an equilibrium interlayer binding energy in good agreement with most recent experiments. We also analyze the behavior of the total energy as a function of interlayer separation at large distances comparing the results with the predictions of the random phase approximation. We then estimate the ratio between exfoliation and binding energy.

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