Séminaire :

“A benchmark for layer cohesion energetics in graphitic systems, via the Random Phase Approximation”

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Résumé :

Systems and nanostructures built on graphene layers are important in various emerging technologies. The cohesion of graphitic layers occurs primarily via dispersion forces. It has recently been shown analytically that these forces have an unusual asymptotic behaviour at large graphene layer separations \( D \) (\( E \propto -D^{-3} \) for \( D \to \infty \) at \( T=0K \)). This behaviour is not captured by common theories that sum \( R^{-6} \) contributions, nor by theories of the “VdW-DF” type. The dispersion energies near the equilibrium layer spacing \( D \approx D_0 \) are however not accessible by purely analytic means, and their value in this regime has been controversial for some years, with sparse and inconsistent experimental data and no credible theoretical values. Because of the importance of graphitic systems, a reliable benchmark is urgently needed. Here we report very recent work using the Adiabatic Connection Fluctuation Dissipation Theorem within the Direct Random Phase Approximation, carried through to numerical convergence without further approximation. This has been applied to the layer binding energy curve of graphite at all separations including near to equilibrium. A benchmark binding energy is thus obtained. This will be compared with very recent work via vDW-DF and Diffusion Monte Carlo methods.