Séminaire LCT/IP2CT

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Correlations in density functional theory

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Despite many recent innovations, some types of electronic correlations remain difficult to treat in DFT. On the one hand, dynamic correlations cause the attractive van der Waals force, which remains difficult to calculate accurately, efficiently, or both.
This is especially true in interesting "low-D" systems such as MoS_2 and van der Waals heterostructures.
On the other hand, degenerate and near-degenerate systems, such as dissociated open shell molecules, pose both practical and conceptual issues.
In this talk I will discuss some of these matters, and (hopefully) present some solutions.