The PLUMED plugin and free energy methods in electronic-structure-based molecular dynamics

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Free energy calculations are relevant to many processes in physical chemistry. Traditionally, within the quantum chemistry community, they have been performed through static approximations that unfortunately present some limits of applicability. Only recently the increase in computing power, codes' scalability, and advances in enhanced sampling techniques are offering new chances to calculate free energies by exploiting explicit sampling of the partition function through molecular dynamics. This extends dramatically the variety of problems that one can tackle and open new avenues, especially in the soft-matter field.
In this talk I will introduce the main concepts of enhanced sampling techniques which are now incorporated into FHI-aims code by means of the open-source PLUMED[1] package.
Some simple examples of typical inputs will be provided and the variety of methods that are available will be illustrated, together with an overview on how to direct the choice towards the most suitable method for the problem under study.

[1] Bonomi, M.; Branduardi, D.; Bussi, G.; Camilloni, C.; Provasi, D.; Raiteri, P.; Donadio, D; Marinelli, F.; Pietrucci, F.; Broglia, R.A.; Parrinello, M. "PLUMED: A portable plugin for free-energy calculations with molecular dynamics", Comp. Phys. Comm. (2009), 180(10), 1961-1972.