From Ab Initio Potential Energy Surfaces to in silico Material Design: Integrating QM Accuracy with HPC Effectiveness

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It becomes increasingly apparent that in new advanced materials, ranging from soft supramolecular networks to complex nano-architectures based on smart responsive processes, molecules are the ultimate "functional" building block to realize such devices. Yet, their rational design calls for a detailed understanding of the atom dynamics in a truly multiscale portrait, a feature unmatched by any singular experimental setup. Thanks to the massive increase of HPC resources, Molecular Dynamics (MD) simulations have the potential to provide such a multi-scale description. The reliability of any MD prediction heavily relies on the accuracy of the employed model potentials, also known as the force-field (FF). Hence, MD success pivots on FF selection. In this framework, the development of robust and automated computational protocols aimed at building FFs only based on first principles is recently attracting a growing attention. Beside the accuracy and intrinsic predictive capabilities of such Quantum Mechanically Derived Force-Fields (QMD-FFs), their straightforward integration with HPC resources through popular MD engines makes them very attractive for *in silico* screening protocols.

A long-lasting effort was devoted in our group to develop efficient QMD-FFs parameterization strategies, which have been implemented in the JOYCE/PICKY protocol. Based on the sole knowledge of the chemical structure of the target compound, QMD-FFs were built and successfully employed to characterize different species, as transition metal complexes or organic dyes for photo-active devices. Here, the whole procedure will be discussed for benchmark yet challenging soft materials in their liquid crystalline phase, where QMD-FFs succeed in yielding a realistic description, well reproducing both a *plethora* of mechanical and thermodynamic properties of the material, and the slow collective self-reorientation process, described and rationalized with atomistic detail.