O.38 pART a pluggin for MEP exploration as a versatile alternative to string approaches

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Finding transition states and diffusion pathways is essential to understand the evolution of materials and chemical reactions. Such characterization is hampered by the heavy computation costs associated with exploring energy landscapes at ab initio accuracy. Here, we present a revisited implementation of the activation-relaxation technique (ARTn) that considerably reduce its costs when used within Density Functional Theory (DFT) energy-force engines. In addition to its competitiveness with respect to string approaches in the context of DFT, this new pluggin allows, in general, an easier integration and porting on several energy-forces engines, an enhanced maintenance and extension capabilities, and a simpler use. The implementation of the pluggin has required an algorithmic revisitation of Lanczos that will be briefly presented. For the moment he pluggin is interfaced with Quantum ESPRESSO. An interface with LAMMPS is in progress. We will show the application on few benchmark examples and compare the accuracy and number of force calculations with Climbing Image Nudged Elastic Band Method (CI-NEB).

We will also discuss the possibility to interface pART with ABINIT and further potential collaboration routes within the development activities of the group.