

# Metadynamics simulations of phase transitions in crystalline and amorphous ices

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Using Molecular Dynamics (MD) to simulate phase transitions is a challenging task due to the big gap between the physical timescales the ones accessible to simulations. Among the different MD accelerating techniques, metadynamics [1] provides a powerful tool to overcome such limitation and to reconstruct the free-energy landscape. The definition of a suitable collective variable tracking the transition mechanism is the key problem and it is strongly process-dependent. Since, in general, phase transitions encompass both short-range chemical changes and long-range collective processes, finding good coordinates is highly non-trivial.

We propose a definition that combines the Path Collective Variable (Path-CV) [2] and the Permutation Invariant Vector (PIV) [3]. This allows to trace a continuous path between the two phases in a two-dimensional space and accounts for the topological complexity of the structures through the PIV metrics. We apply such methodology to different phase transitions between crystalline and amorphous ice phases, exploring the mechanisms and energetics of the processes at different thermodynamics conditions (pressure and temperature) by computing free-energy barriers and transition paths [4].

## Bibliography

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