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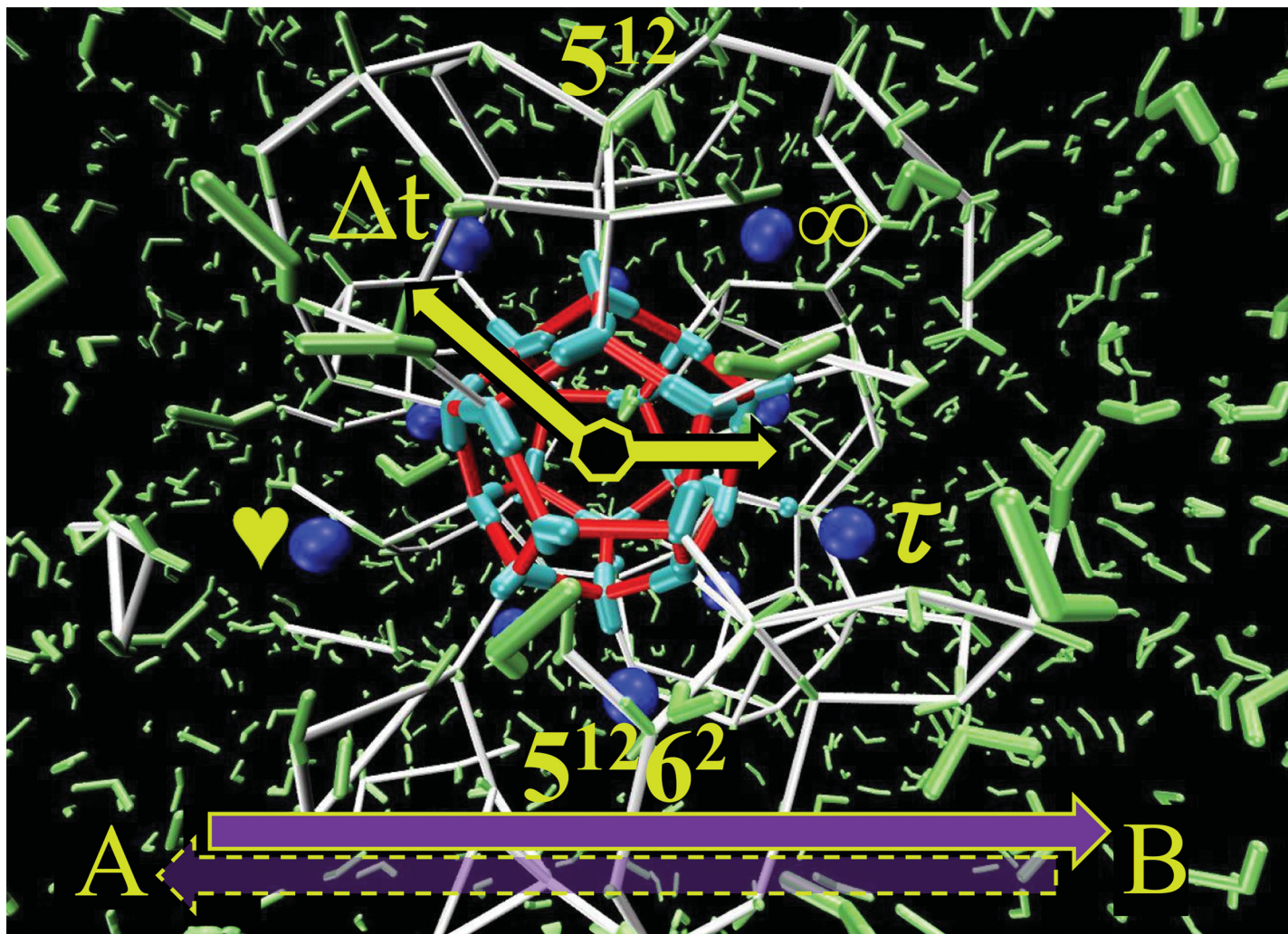
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Showcasing a perspective from Matthew R. Walsh,
Equation 1 LLC, Mishawaka, IN

Comparing brute force to transition path sampling for gas hydrate nucleation with a flat interface: comments on time reversal symmetry

Nucleation is not reversed melting. Brute force explores crystalline trajectories before transition path sampling as driving force is reduced. Image: Hydrate clock with main cages in crystalline (vs. amorphous) reaction coordinate, the times opposite each other, and the infinitely long crystalline brute force result opposite the sometimes-amorphous core in transition path ensemble.

Image generated using Visual Molecular Dynamics (Humphrey, W., Dalke, A. and Schulten, K., "VMD - Visual Molecular Dynamics", J. Molec. Graphics, 1996, vol. 14, pp. 33-38)

As featured in:



See Matthew R. Walsh,
Phys. Chem. Chem. Phys.,
2024, **26**, 5762.