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# 【515】Silicon liquid structure and crystal nucleation from ab-initio deep metadynamics

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We trained a deep neural network potential [1] based on a set of data generated by well-tempered metadynamics [2] simulations that use a classical potential.
We employed the SCAN exchange-correlation functional [3] and converged the calculations with respect to BZ sampling.
The resulting potential is used to study the nucleation and liquid state properties of silicon, on timescales and system sizes that are beyond the reach of ab-initio molecular dynamics.

*[1] Zhang, E et al., P.R.L. (2018)*
*[2] Barducci, Bussi, and Parrinello, P.R.L. (2008)*
*[3] Sun, Ruzsinszky, and Perdew, P.R.L. (2015)*

**Primary authors:** BONATI, Luigi (ETH Zurich and USI Lugano); Prof. PARRINELLO, Michele (ETH Zurich and USI Lugano)

**Presenter:** BONATI, Luigi (ETH Zurich and USI Lugano)

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