

# Crystal structure prediction of La-H high-pressure hydrides with account of anharmonicity

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Accounting the anharmonic nature of free energy landscape within the stochastic self-consistent harmonic approximation (SSCHA) in hydrides can improve predictions of their stability and correctness of determining their crystal structure facilitating the search for new hydride superconductors. However, fully ab initio-based calculations of the anharmonic free energy within SSCHA is computationally very intensive task that makes unfeasible taking the anharmonicity into account in the theoretical crystal structure searches where the free energies of thousands of candidate structures should be calculated. To overcome this challenge, we propose the use of moment-tensor potentials (MTP) in conjunction with USPEX and SSCHA illustrating this approach on the example of the La-H system.