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Liquid Metal Free Energies from Ab Initio Potential Surfaces CARL GREEFF, RAQUEL LIZARRAGA, ERIC CHISOLM, Los Alamos National Laboratory — For prediction of high pressure melting curves and liquid thermodynamic properties, it is desirable to evaluate liquid free energies. Direct free energy calculations from *ab initio* potential surfaces are very computationally intensive, especially for transition metals. Here we investigate Monte Carlo methods that involve sampling on the surface defined by a reference system. In principle, this allows for large gains in efficiency because the random walk is carried out on the (much faster) reference potential, and the *ab initio* potential is only evaluated on a small subset of uncorrelated configurations. We investigate the feasibility of these methods, and the role of the reference system. Results will be presented for liquid Mg and Ta.

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