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Free energies from ab initio calculations for liquid Mg RAQUEL LIZARRAGA, Universidad Austral de Chile, CARL GREEFF, Los Alamos National Laboratory — We performed free energy calculations for liquid metals from *ab initio* potential surfaces by means of Monte Carlo methods that involve sampling on the potential surface defined by a reference system. 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. This is highly desirable since direct free energy calculations for liquid metals from ab initio potential surfaces are very computationally intensive. Our calculations on liquid magnesium shows that we can obtain free energies accurate at the meV/atom level with only 100 evaluations of the *ab initio* total energies.

Raquel Lizarraga
Universidad Austral de Chile

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