**Exploring HP protein models using Wang-Landau sampling**
THOMAS WUEST, DAVID P. LANDAU, The University of Georgia, USA — The hydrophobic-polar (HP) protein model has become a standard in assessing the efficiency of computational methods for protein structure prediction as well as for exploring the statistical physics of protein folding in general. Numerous methods have been proposed to address the challenges of finding minimal energy conformations within the rough energy landscape of this lattice heteropolymer model. However, only a few studies have been dedicated to the more revealing - but also more demanding - problem of estimating the density of states which allows access to thermodynamic properties of a system at any temperature. Here, we show that Wang-Landau sampling, in connection with a suitable move set ("pull moves"), provides a powerful route for the ground state search and the precise determination of the density of states for HP sequences (with up to 100 monomers) in both, two and three dimensions. Our procedure possesses an intrinsic simplicity and overcomes the inevitable limitations inherent in other more tailored approaches. The main advantage lies in its general applicability to a broad range of lattice protein models that go beyond the scope of the HP model.

Thomas Wuest
The University of Georgia, USA

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