Amgen Seminar Series in Chemical Engineering

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Good + Bad = Ugly, and other pitfalls to avoid when calculating free energies

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Molecular simulation is an experiment performed on a system defined by a molecular model. In recent years much of the effort to advance molecular simulation has been put toward improving the quality and quantity of information that it provides. These efforts have been very successful, and perhaps have improved the utility of molecular simulation even more than advances in raw computing power occurring over the same period. One important application of molecular simulation is the calculation of free-energy differences, which are required for analyses of phase and reaction equilibria, solvation, binding affinity, stability, kinetics, and so on. Some of the most popular approaches to calculating the free energy are highly prone to systematic errors, and simple countermeasures designed to remedy these inaccuracies often do not improve the outcome. We show that the key consideration influencing the accuracy is the overlap of the important regions of phase space for the systems of interest. We are developing measures to quantify this overlap and we examine the connection between them and the performance of the calculations. We use these ideas to formulate simple variants of the basic technique that can be applied to increase the likelihood of obtaining a good result.

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