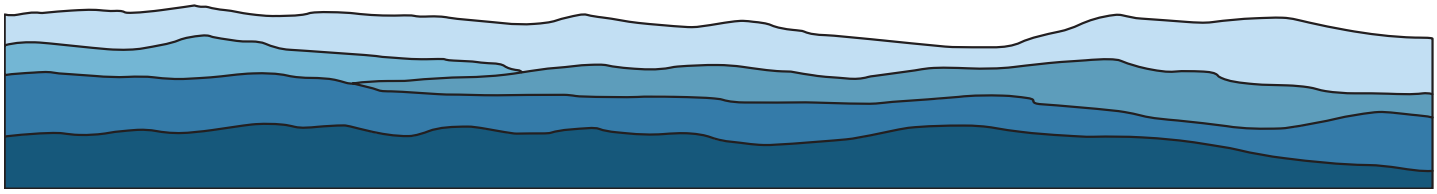
HIGHLANDS IN CHEMISTRY SEMINAR SERIES



QIANG CUI

BOSTON UNIVERSITY

"Exploration of machine learning methods and the effect of electronic polarization in biomolecular simulations"

APRIL 19, 2024

2:30PM

HAHN HALL NORTH 140

FACULTY HOST:
VALERIE WELBORN

I'll first discuss several recent studies in the group that explored the use of machine learning methods in biomolecular simulations. These include the use of reinforcement learning to construct high-dimensional free energy surfaces and approaches for improving the accuracy of semi-empirical QM/MM free energy simulations by learning how a semi-empirical QM/MM potential function differs from a high-level QM/MM model. In a separate line of work, we also explored the use of machine learning methods to aid the determination of lipid phase transition temperature in the context of generalized replica exchange molecular dynamics simulations. Finally, I'll also discuss our exploration of including electronic polarization in the description of protein cavity hydration. We implemented a grand canonical non-equilibrium candidate Monte Carlo approach to predict cavity hydration in proteins using polarizable force fields. Even for a relatively solvent accessible polar cavity in trypsin, including electronic polarization leads to a modest but clear improvement on the description of binding pocket hydration. The hydration levels of the dewetted state of the central cavity in the Big Potassium Channel are observed to be substantially different with polarizable and non-polarizable models, suggesting that an accurate treatment of hydrophobic gating of ion channels and transporters requires the inclusion of electronic polarization.

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