



Software Framework for Electronic Structure of Molecules and Solids

Garnet Kin-Lic Chan

Caltech

Toru Shiozaki



Northwestern
University



QSIMULATE

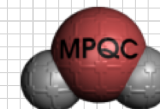
Edward F. Valeev



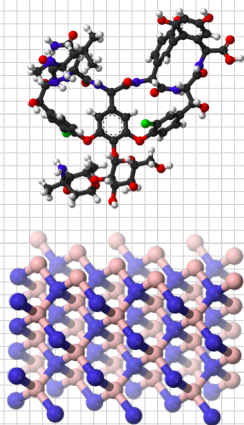
VIRGINIA
TECH.



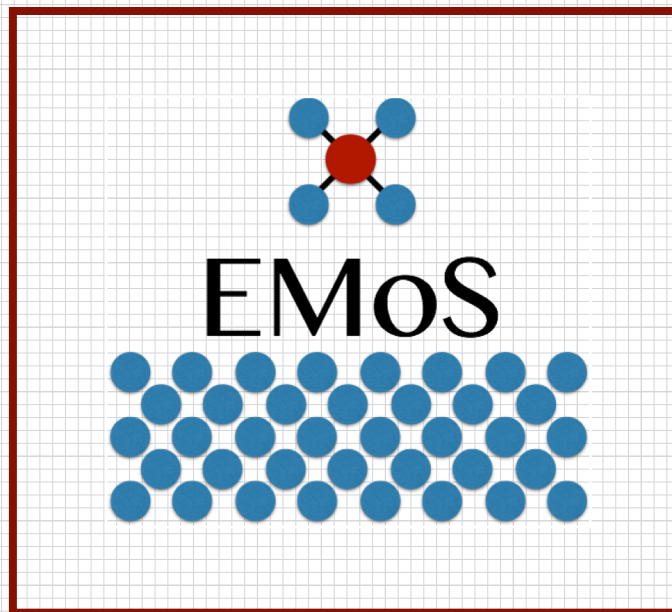
BAGEL



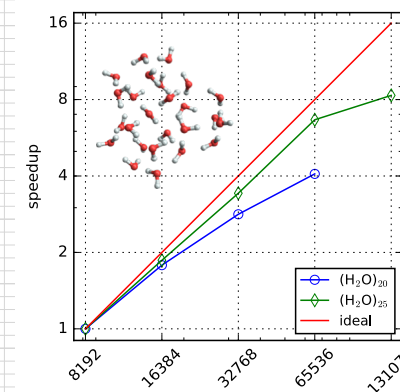
molecules and solids



reduced complexity formalisms



high-level composition in C++/Python



high performance with 1 ... 10⁵ cores