

QM/MM concepts

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- System separation in a QM/MM simulation

- Additive and subtractive schemes

- Mechanical embedding and Electrostatic embedding

- Treatment of covalent bonds at the boundaries

- NAMD + GAUSSIAN

Resources

NAMD Hybrid QM/MM

<http://www.ks.uiuc.edu/Research/qmmm/>

Martin Karplus article:

<http://onlinelibrary.wiley.com/doi/10.1002/jcc.540110605/abstract>

Walter Thiel:

http://link.springer.com/chapter/10.1007/128_2006_084

Recent review from Qiang Cui:

10.1021/acs.jpcc.0c09898