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Construction of Coarse Grained Rigid Blob- Small Oscillation Model

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Recently the advances on improving the algorithms of multiscale computation methods have become a front-line research topic. We have extended the previously developed coarse grained rigid blob (CGRB) model [1], together with the on-going quantum chemistry calculations, to construct an improved coarse grained model based on these ab initio data. In contrast to our previous CGRB model, we introduce the small oscillation approximation in order to model the low frequency intramolecular vibrational modes and the effect on intermolecular force fields. We derive the analytical formula and implement the formula into our molecular dynamics simulation program. We apply this new methodology to an acute polymer (PNIPAM) system and study the dynamical properties.

REFERENCES

[1] S. D. Chao, J. D. Kress and A. Redondo, Coarse-grained rigid blod model for soft matter simulations. *J. Chem. Phys.*, Vol. **122**, pp. 234912/14, 2005.