

Supplementary Materials For

Modeling Viscoelastic Relaxation Dynamics of Soft Particles via Molecular Dynamics Simulation-Informed Multi-Dimensional Transition-State Theory

Shangchao Lin^{1,†}, Lingling Zhao^{2,3,†,*}, Shuai Liu², Yang Wang², Ge Fu¹

¹Institute of Engineering Thermophysics, School of Mechanical Engineering, Shanghai Jiao Tong University, Shanghai, 200240, China

²Key Laboratory of Energy Thermal Conversion and Control of Ministry of Education, School of Energy & Environment, Southeast University, Nanjing, Jiangsu, 210096, China

³Shanghai Key Laboratory of Multiphase Flow and Heat Transfer in Power Engineering, University of Shanghai for Science and Technology, Shanghai, 200093, China

*Corresponding author's contact information:

Lingling Zhao, phone: +86 13851680995; E-mail: zhao_lingling@seu.edu.cn

[†]These authors contribute equally to this work.

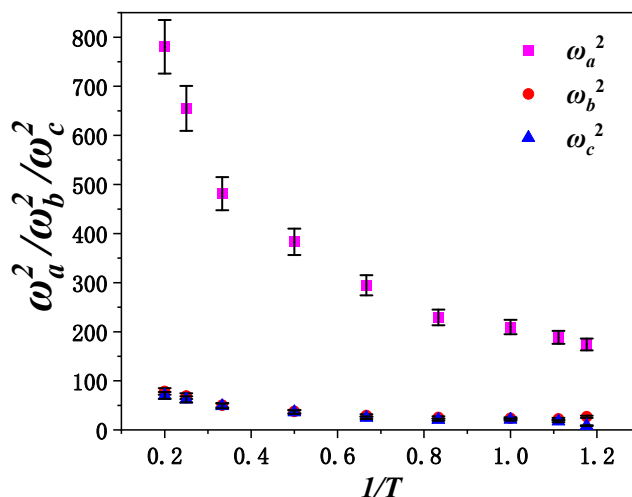


Figure S1. The squared angular frequencies ω_a^2 , ω_b^2 and ω_c^2 for the single particle type system. The error bars reflect the standard deviations from averaging three replicated MD simulation runs.

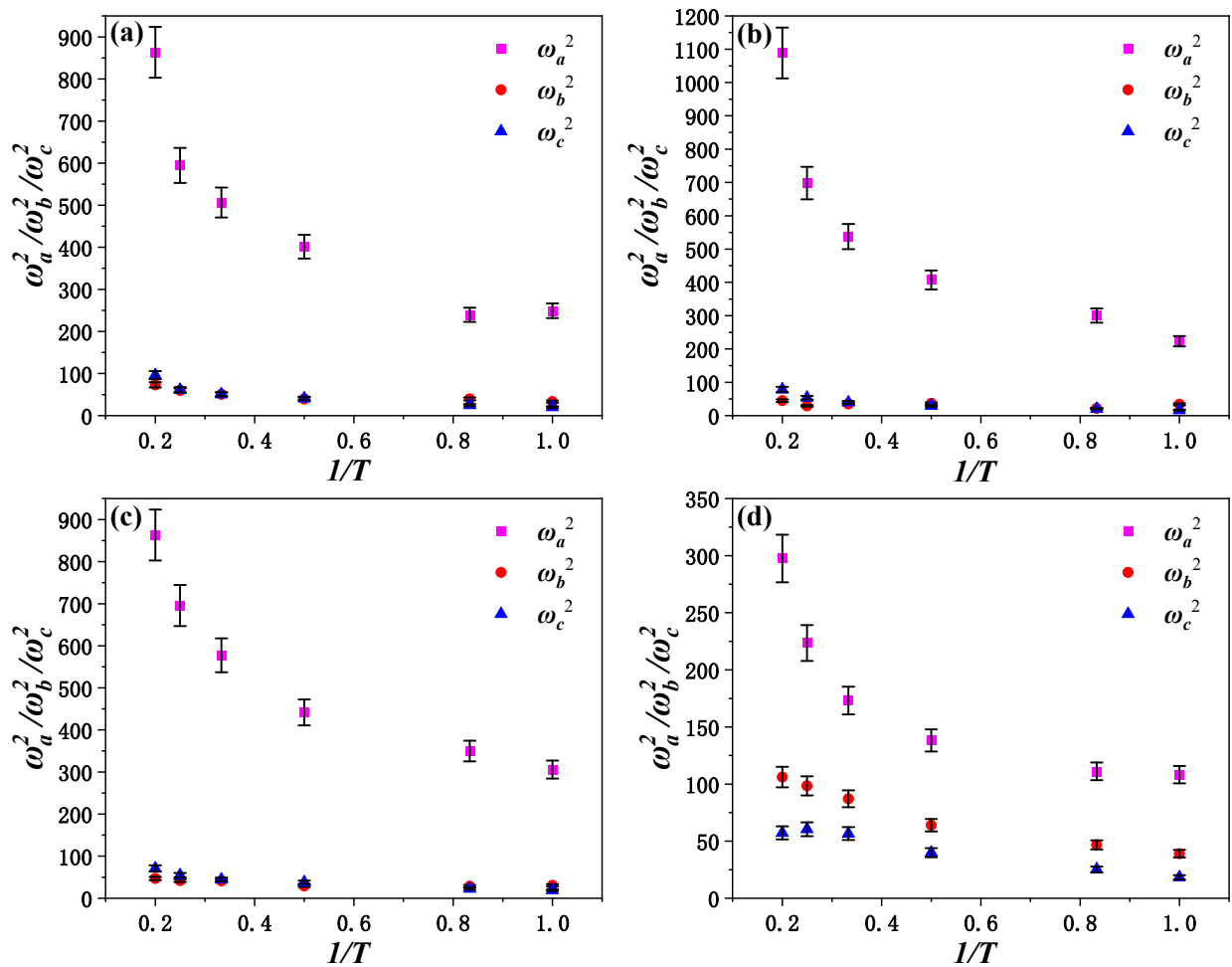


Figure S2. The squared angular frequencies ω_a^2 , ω_b^2 and ω_c^2 for the binary mixture KA system between: (a) A-A pair, (b) B-B pair, (c) A-B pair, and (d) all-all pair. The error bars reflect the standard deviations from averaging three replicated MD simulation runs.

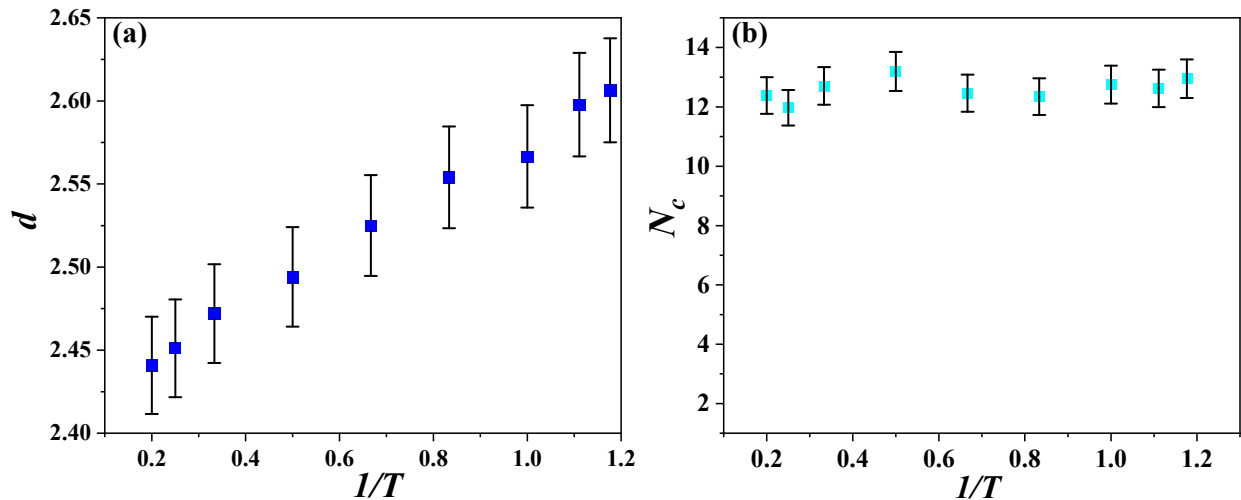


Figure S3. (a) The fractal dimension d and (b) coordination number N_c for the single particle type LJ system. The error bars reflect the standard deviations from averaging three replicated MD simulation runs.

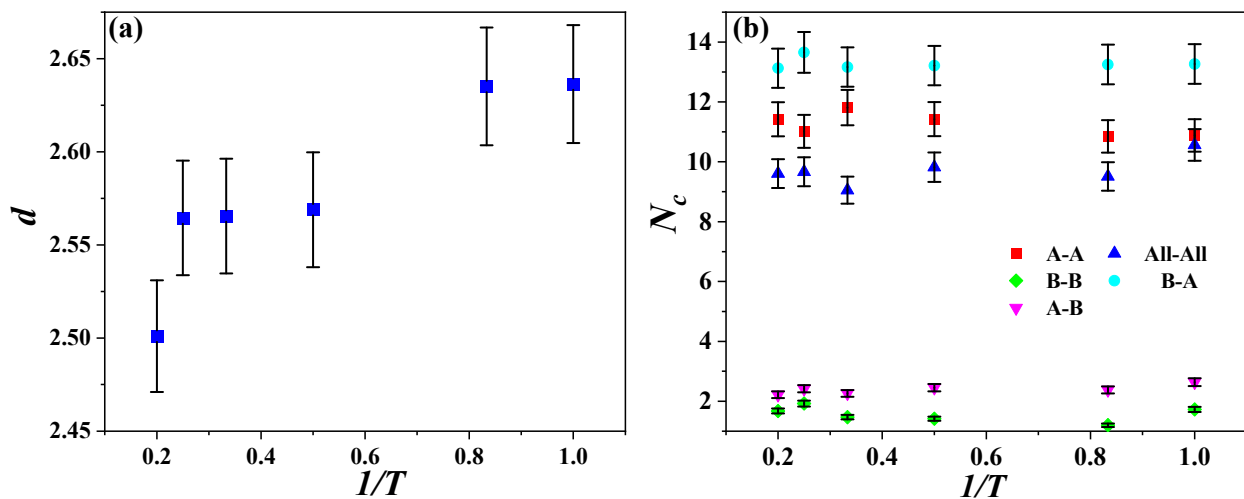


Figure S4. (a) The fractal dimension d and (b) coordination number N_c for the binary mixture KA system. The error bars reflect the standard deviations from averaging three replicated MD simulation runs.