Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Liquid-like properties of cyclopentadienyl complexes of barium: Molecular dynamics simulations of nanoscale droplets

Hye Ree Hyun[a†], Jungim Han[b†], Juhyung Lim[b], Young Jae Park[b], Byoungki Choi[b],

Chul Baik[b*], and Jun Soo Kim[a*]

[a]Department of Chemistry and Nanoscience, Ewha Womans University, Seoul 03760, Republic of Korea

[b]Organic Material Lab, Samsung Advanced Institute of Technology, Suwon, Gyeonggi-do 16678, Republic of Korea

* Corresponding author: jkim@ewha.ac.kr, chul.baik@samsung.com

† These authors contributed equally to this work

Contents

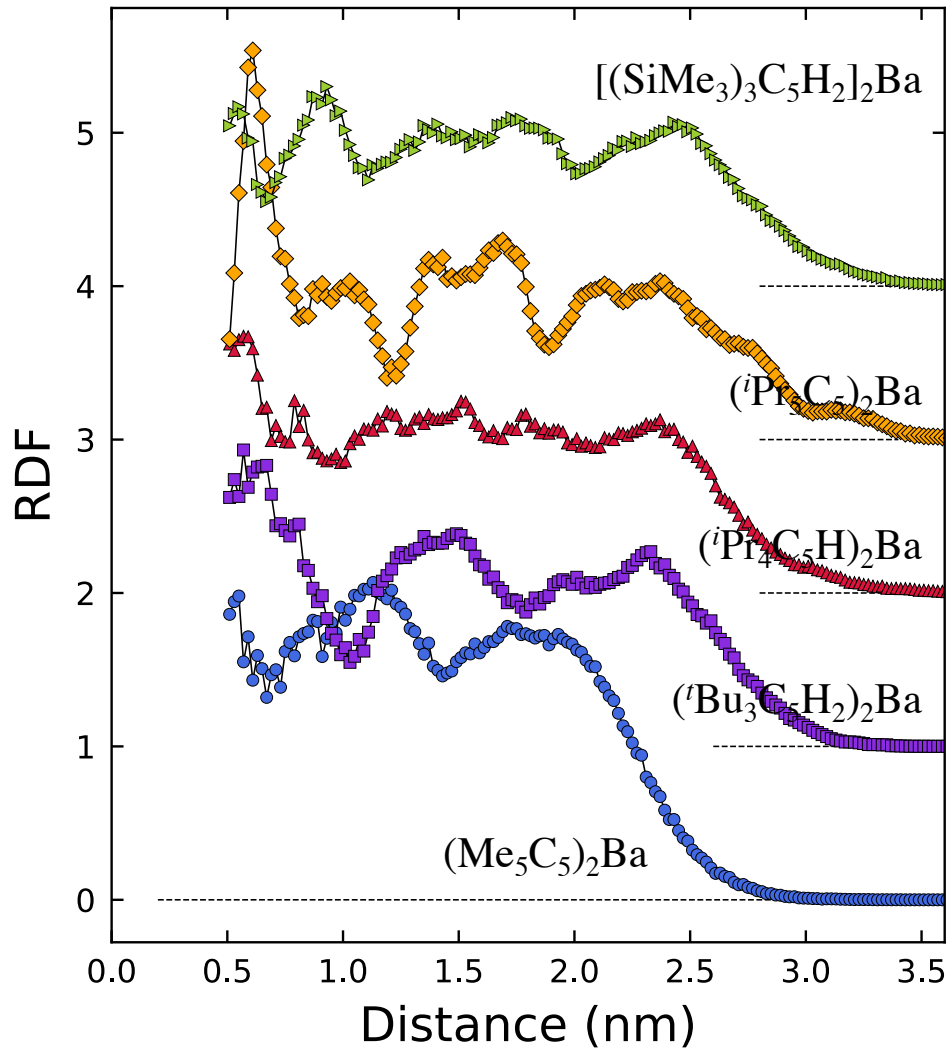

Fig. S1. Comparisons of radial density profiles around a center-of-mass of each droplet. The density profiles are fitted to hyperbolic tangent functions, $\rho(r) \sim \tanh\frac{(r_d - r)}{\delta}$, to determine the droplet radius r_d as an inflection point of the density decrease to zero and the interfacial thickness 2δ. The density profiles are shifted vertically for visual clarity.

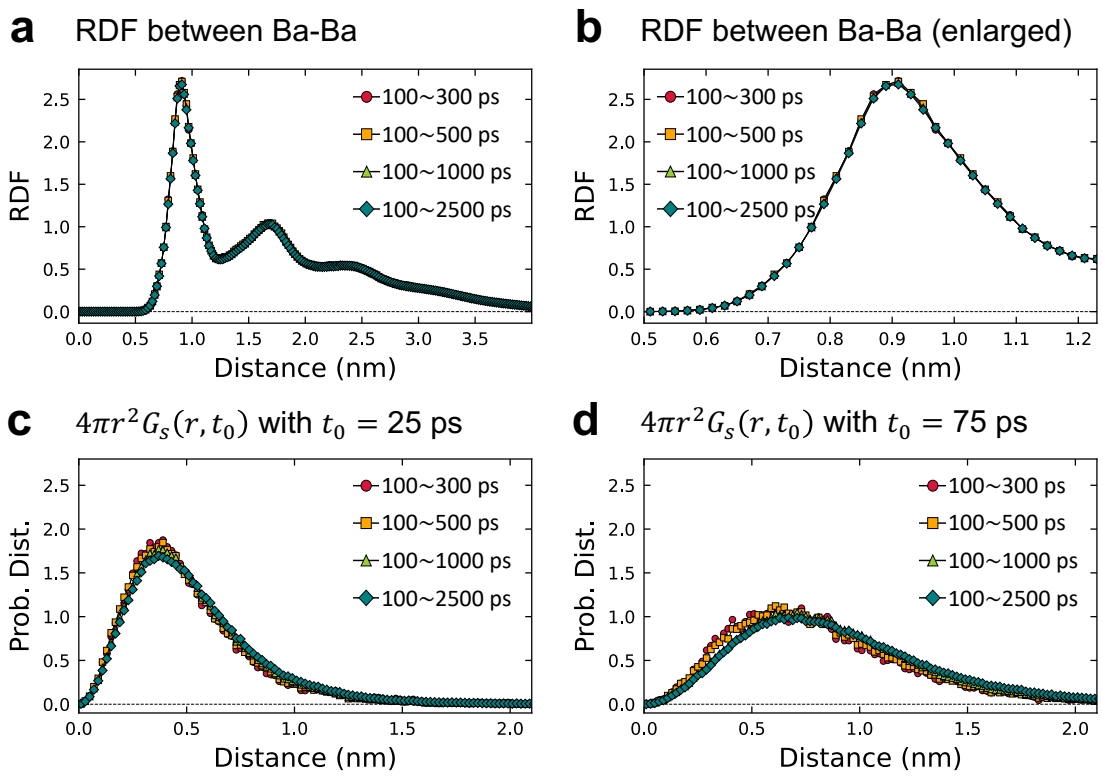

Fig. S2. Comparisons of structural and dynamic properties of a nanoscale droplet composed of 96 molecules of $(Me_5C_5)_2Ba$ calculated during different simulation durations. (A) Radial distribution functions (RDF) between central Ba atoms calculated for various simulation times. (B) Enlarged view of the first RDF peak presented in (A). (C) and (D) Radial probability distributions of particle displacements within time intervals of $\boldsymbol{t_0}$ = 25 ps and 75 ps, respectively. These were calculated between the simulation times indicated in the figure. $\boldsymbol{G_s(r, t_0)}$ is the self part of the van Hove correlation function, where $\boldsymbol{r}$ is particle displacement and $\boldsymbol{t_0}$ is the time interval for displacements. Except for small deviations of the van Hove correlation function at durations of 200 and 400 ps, all data in (A)-(D) agree very well with each other. This suggests that simulation duration > 400 ps is sufficient for providing reliable data for structural and dynamic properties.

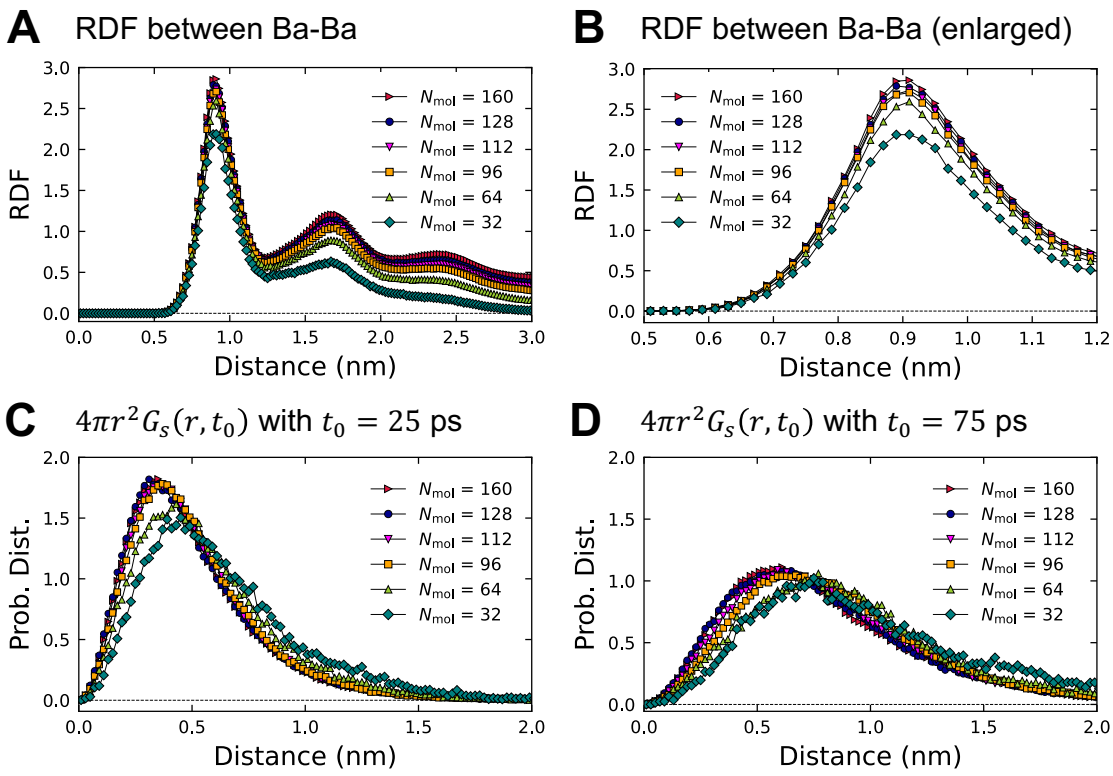

Fig. S3. Comparisons of structural and dynamic properties of nanoscale droplets of $(Me_5C_5)_2Ba$ calculated from simulations with different numbers of molecules composing the droplet. (A) Radial distribution functions (RDF) between central Ba atoms calculated from simulations with 32 to 160 molecules N_{mol}. (B) Enlarged view of the first RDF peak presented in (A). (C) and (D) Radial probability distributions of particle displacements within time intervals of $\boldsymbol{t_0}$ = 25 ps and 75 ps, respectively. These were calculated for different N_{mol} as indicated in the figure. $\boldsymbol{G_s(r, t_0)}$ is the self part of the van Hove correlation function, where $\boldsymbol{r}$ is particle displacement and $\boldsymbol{t_0}$ is the time interval for displacements. The plots in (A)-(D) for different N_{mol} converge as N_{mol} increases. We chose N_{mol} = 96 for the simulations of nanoscale droplets of various complexes presented in the main text, because the results of N_{mol} = 96 agree reasonably well with those of larger droplets while the computation is fast enough for each simulation to be done within about a month. For instance, the 1-ns simulation of 96 molecules of $(^iPr_5C_5)_2Ba$ took 37 days using AMD Ryzen 9 3900X 12-CPU 24-thread processors.

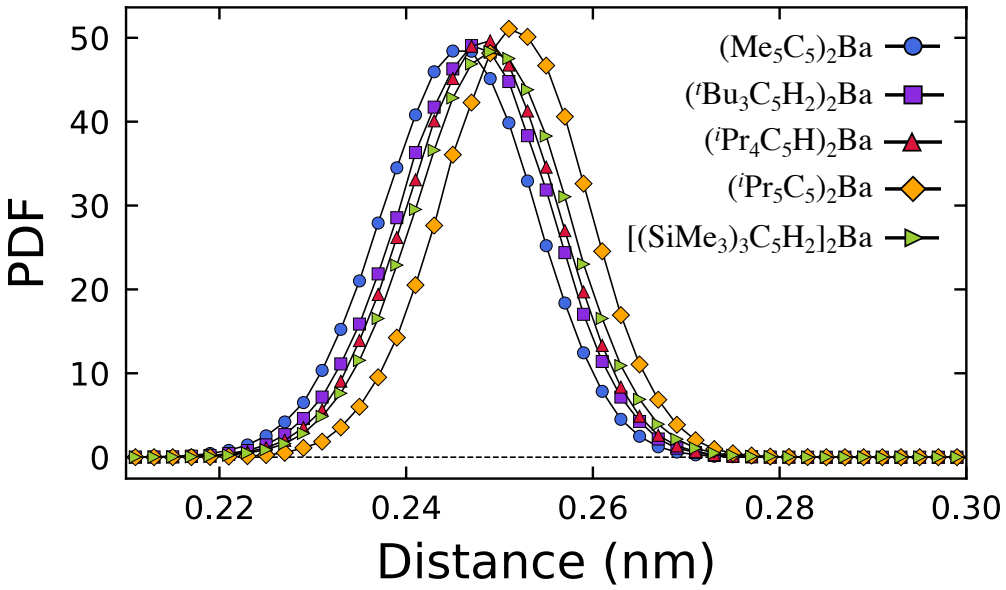

Fig. S4. Probability distribution functions of the distance between a central barium atom and a ligand centroid in each molecule.