Electronic Supplementary Material (ESI) for RSC Advances.

Kinetic Monte Carlo simulations of the assembly of filamentous biomacromolecules by dimer addition mechanism

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Supplementary Materials

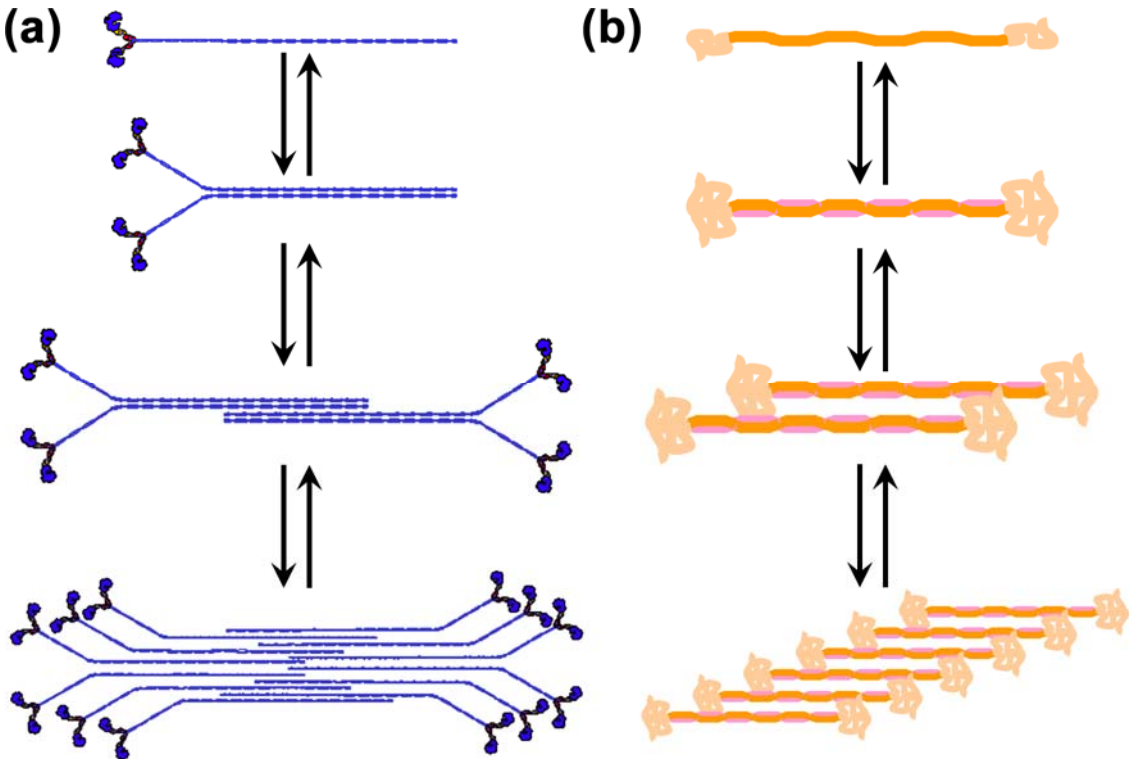

Figure S1. The schematic graph of the assembly of myosin II thick filaments (a) and intermediate filaments (b) through dimer addition, respectively. After the formation of dimer, further assembly proceeds by adding dimer to existing oligomers.

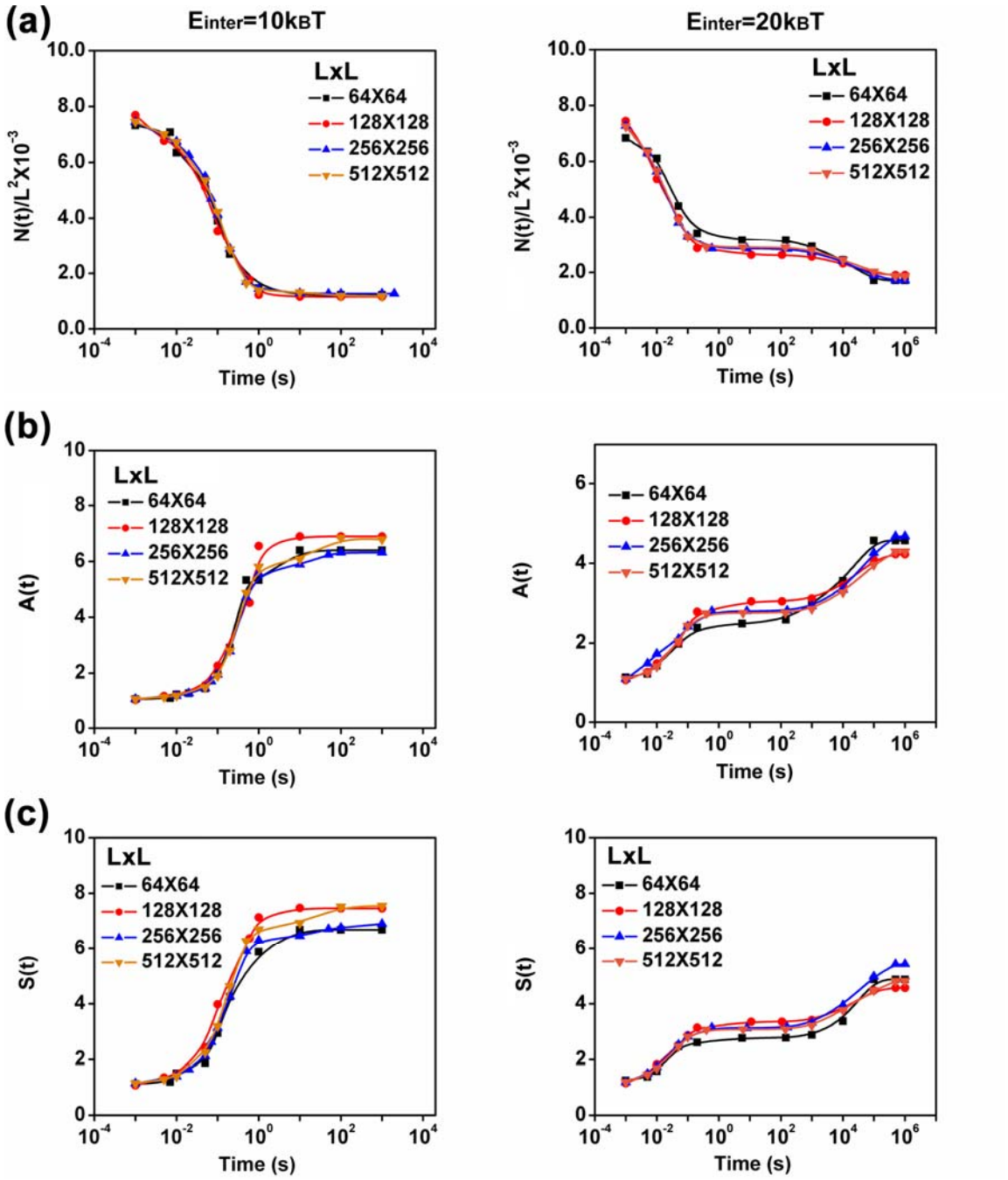

Figure S2. The effect of size of simulation window L×L on the cluster density (a), the number average cluster size (b) and the weight average cluster size (c) is small. Here L has different values of 64, 128, 256 and 512.

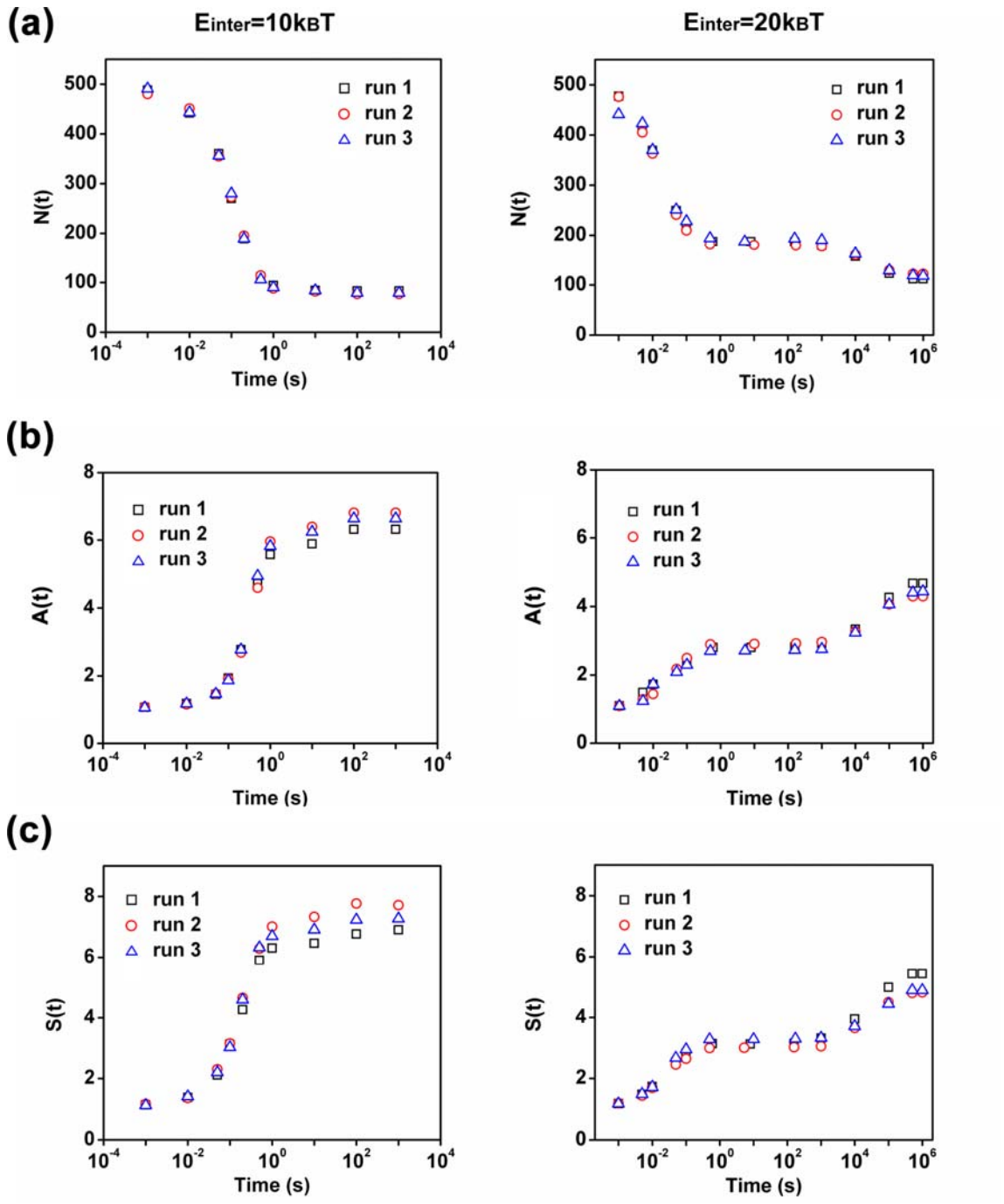

Figure S3. The effect of random seeding on the aggregation of dimmers is negligible. The evolutions of the number of clusters N(t), number average cluster size A(t) and weight average cluster size S(t) are shown in (a), (b) and (c), respectively.

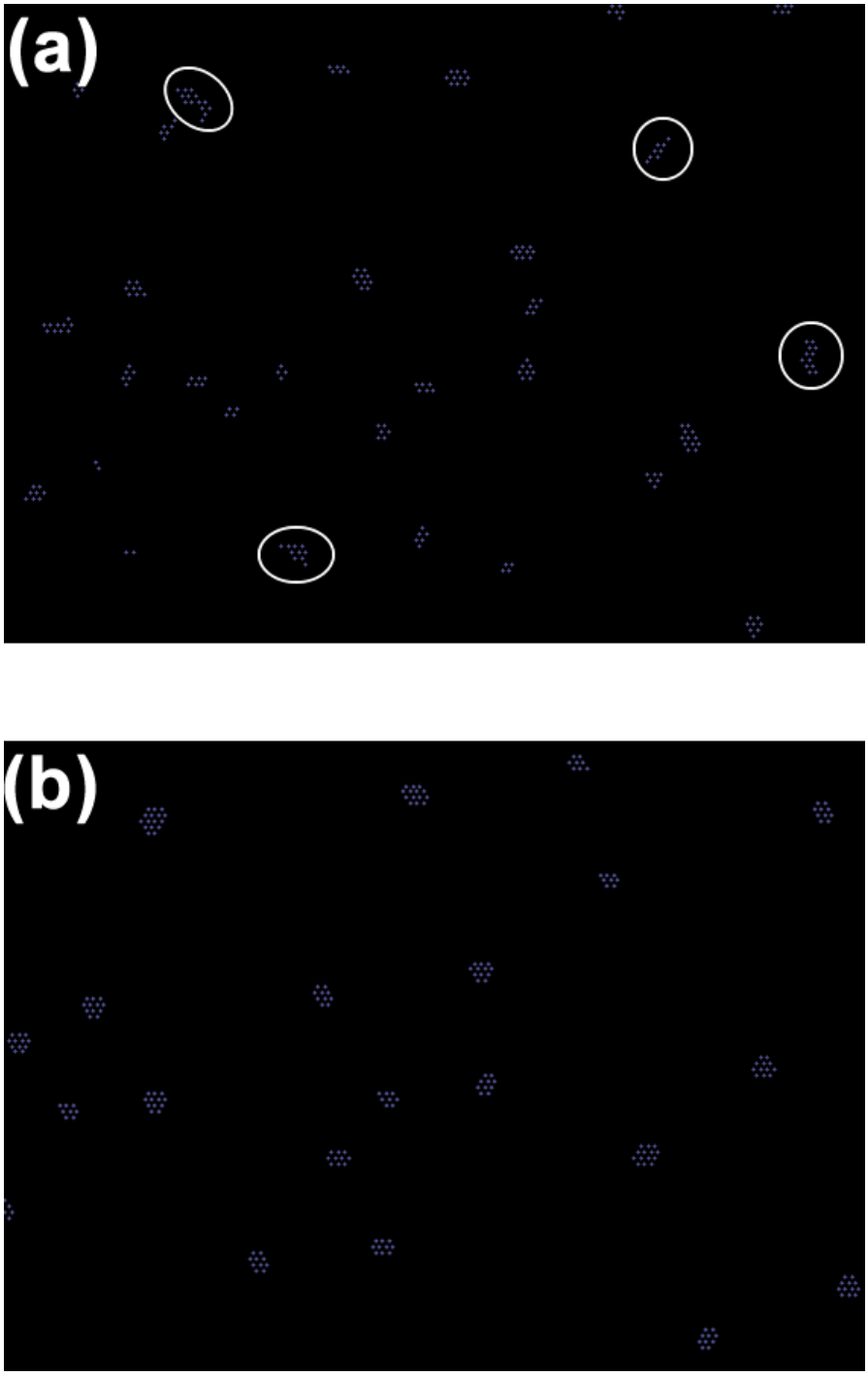

Figure S4. Snapshots of the configurations of oligomers in the intermediate plateau (a) and the steady-state (b) of a double-S shape aggregation where E_{inter}=10 k_BT, Γ_{off} =10^6 Hz, r_{diff}^{mono} =1.0 μm^2/s and φ =0.016. The unstable (uncompacted) clusters in the intermediate plateau are labeled with white circles. Only a small part of the simulation window is shown here.

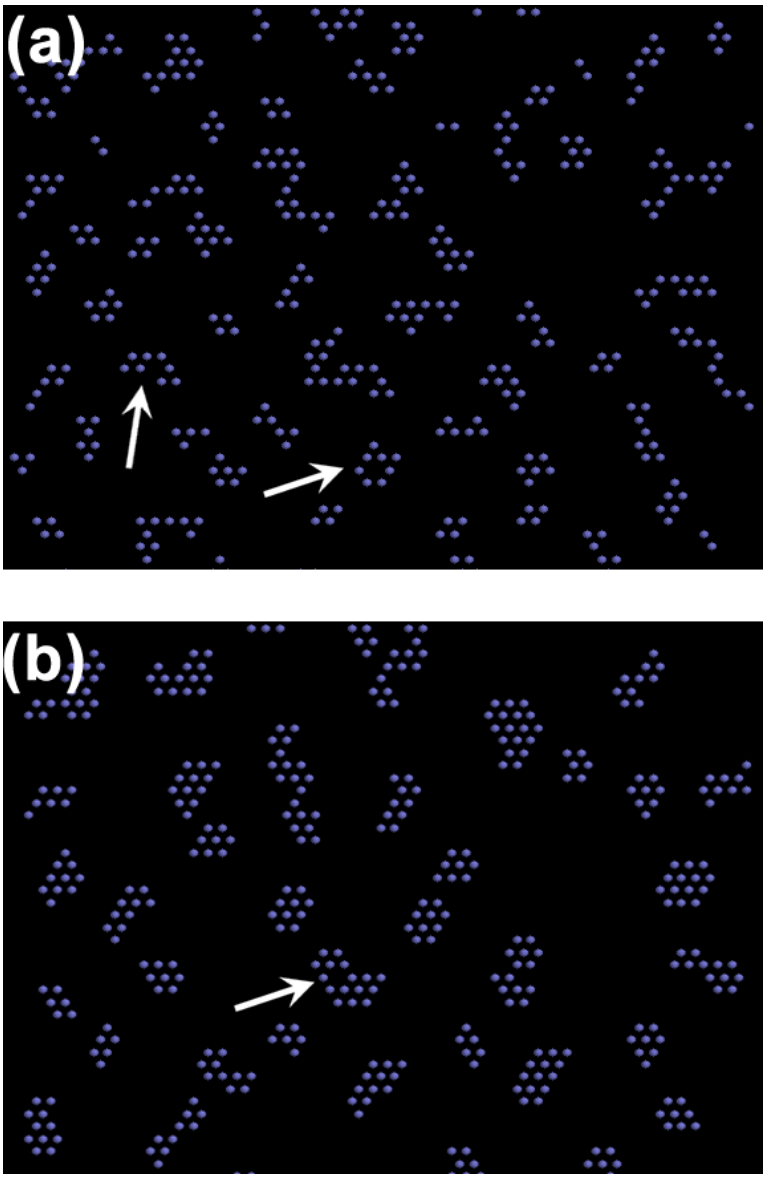

Figure S5. The configurations of oligomers in elary (a) and later (b) stages of aggregations where Γ_{off} =10^6 Hz, E_{inter}=10 k_BT, r_{diff}^{mono} =0.1 μm^2/s and φ =0.16. By comparison, oligomers are more compacted in late stage. Only a small part of the simulation window is shown here.

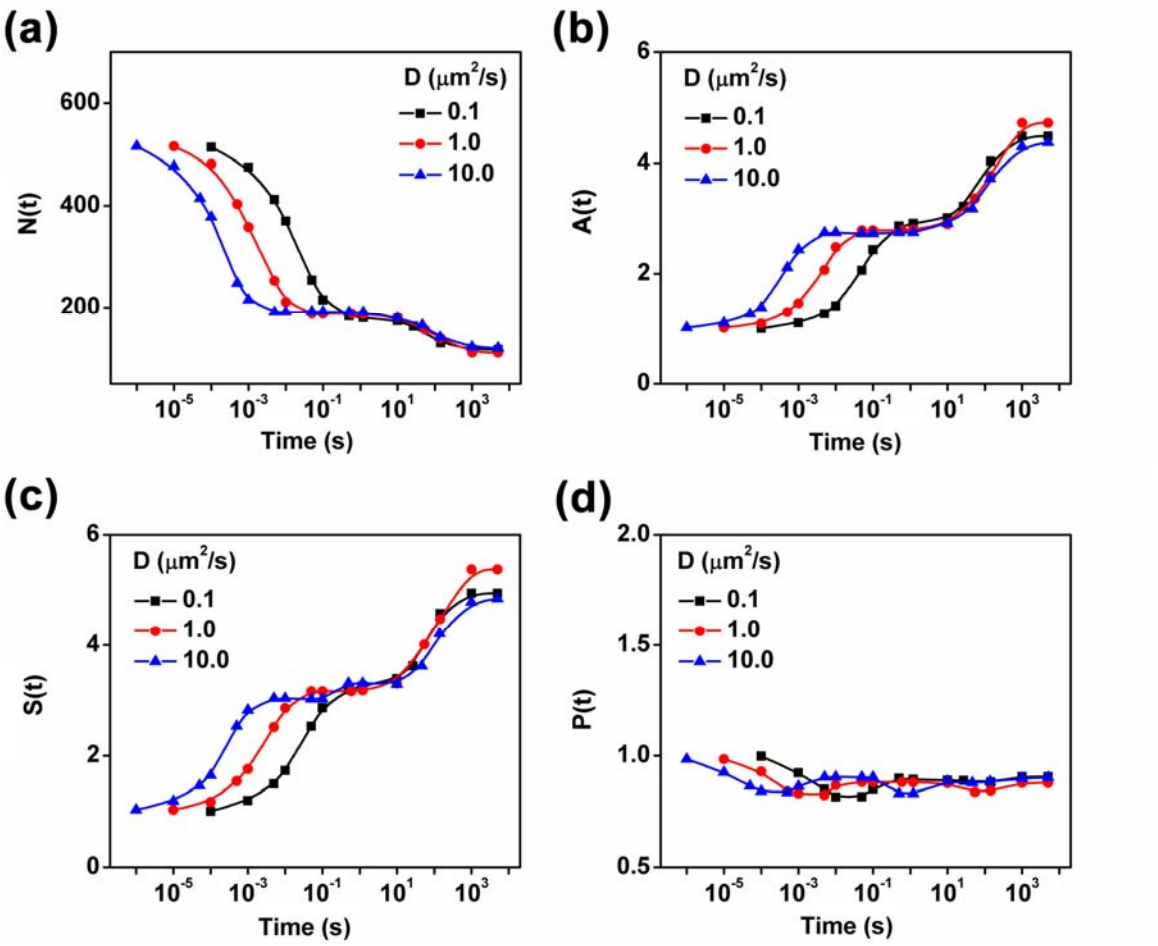

Figure S6. The aggregation kinetics with different diffusion coefficients at r_{diff}^{mono} =0.1 μm^2/s, Γ_{off} =10^4 Hz and φ =0.016.

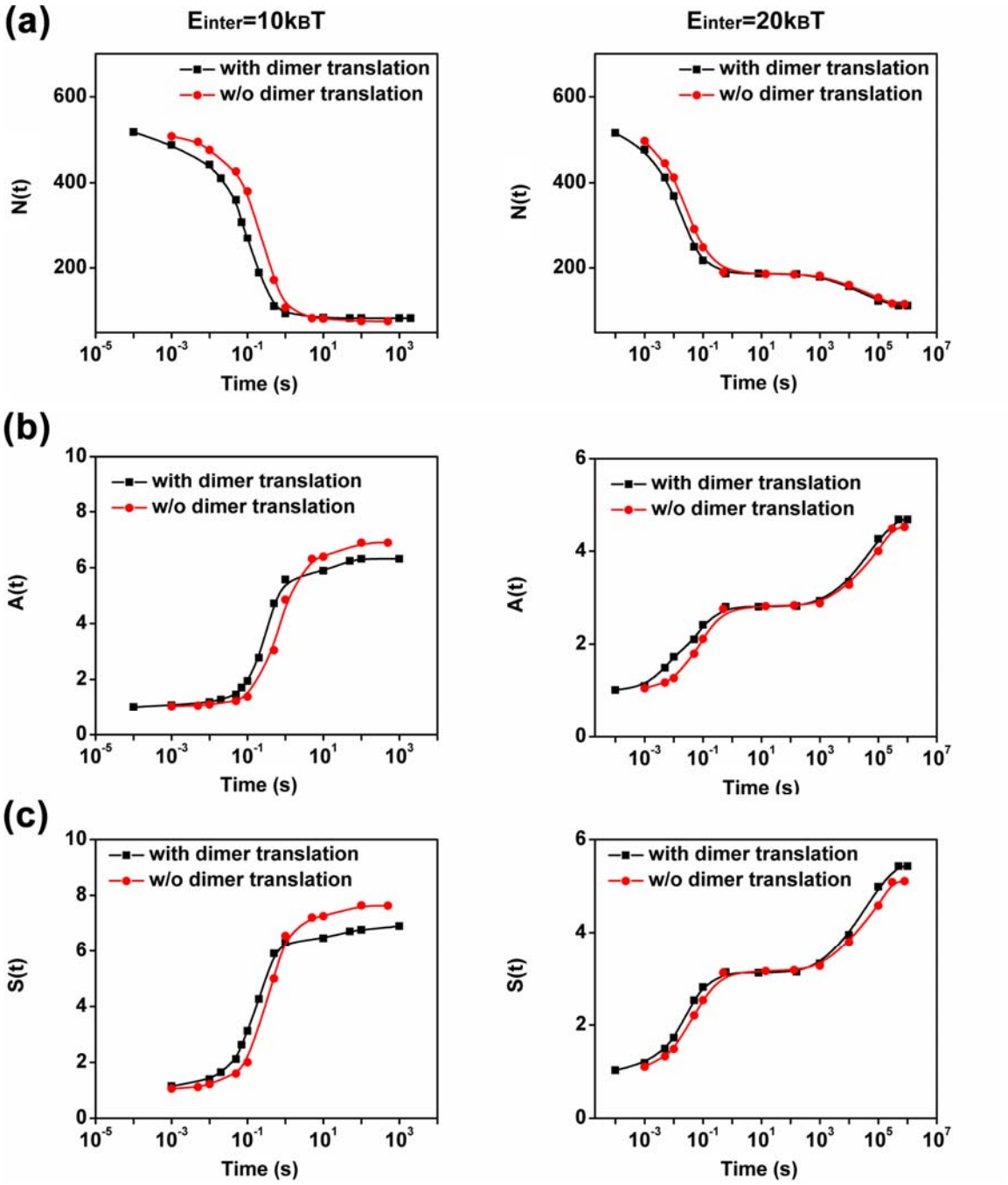

Figure S7. The effect of translation motion of dimers on the aggregation kinetics at r_{diff}^{mono} =0.1 μm^2/s, Γ_{off} =10^6 Hz and φ =0.016.

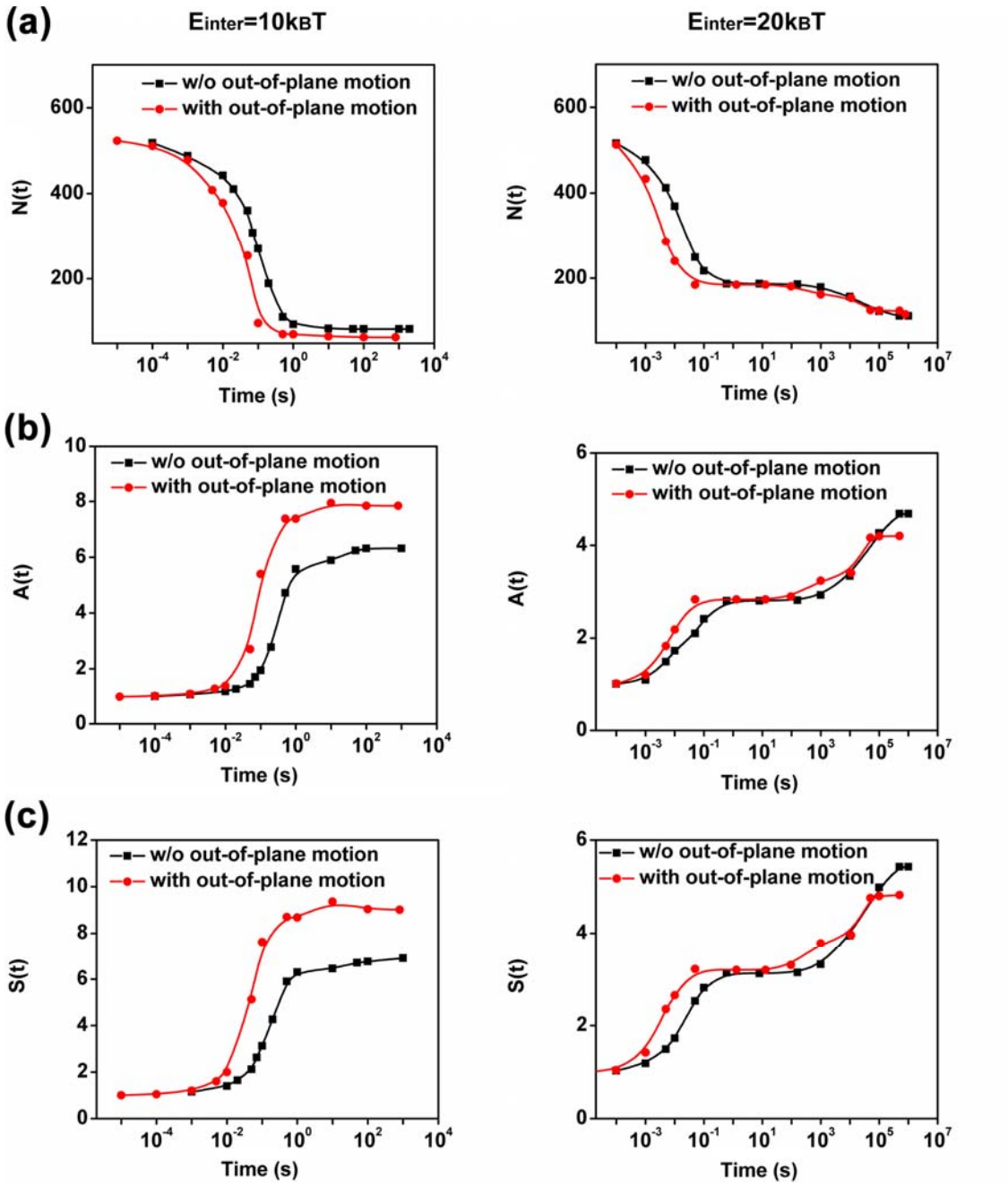

Figure S8. The effect of out-of-plane motion of dimers on the aggregation kinetics. Here, the rates of the out-of-plane motion (in and out) are 10 times of r_{diff}^{mono}. Other pamaters are r_{diff}^{mono}=0.1 μm^2/s, Γ_{off}=10^6 Hz and φ=0.016.