

Figure S1. The relationship among ρ , λ_2 and the interactions when the $Sign(\lambda_2(r))\rho(r)$ function is projected onto the isosurface of RDG function

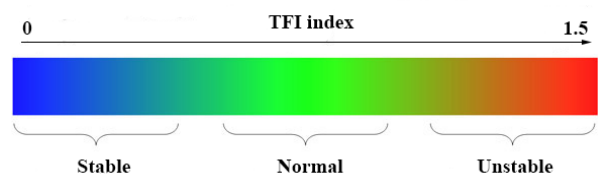


Figure S2. The relationship between TFI index and the stabilities of the interactions when the TFI function is projected onto the isosurface of the RDG function

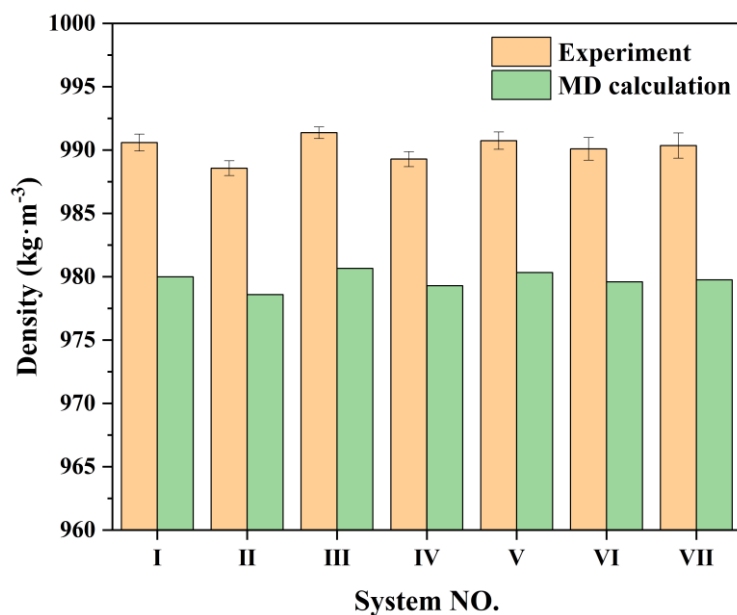


Figure S3. The comparison between the experimental and the simulated densities for different systems

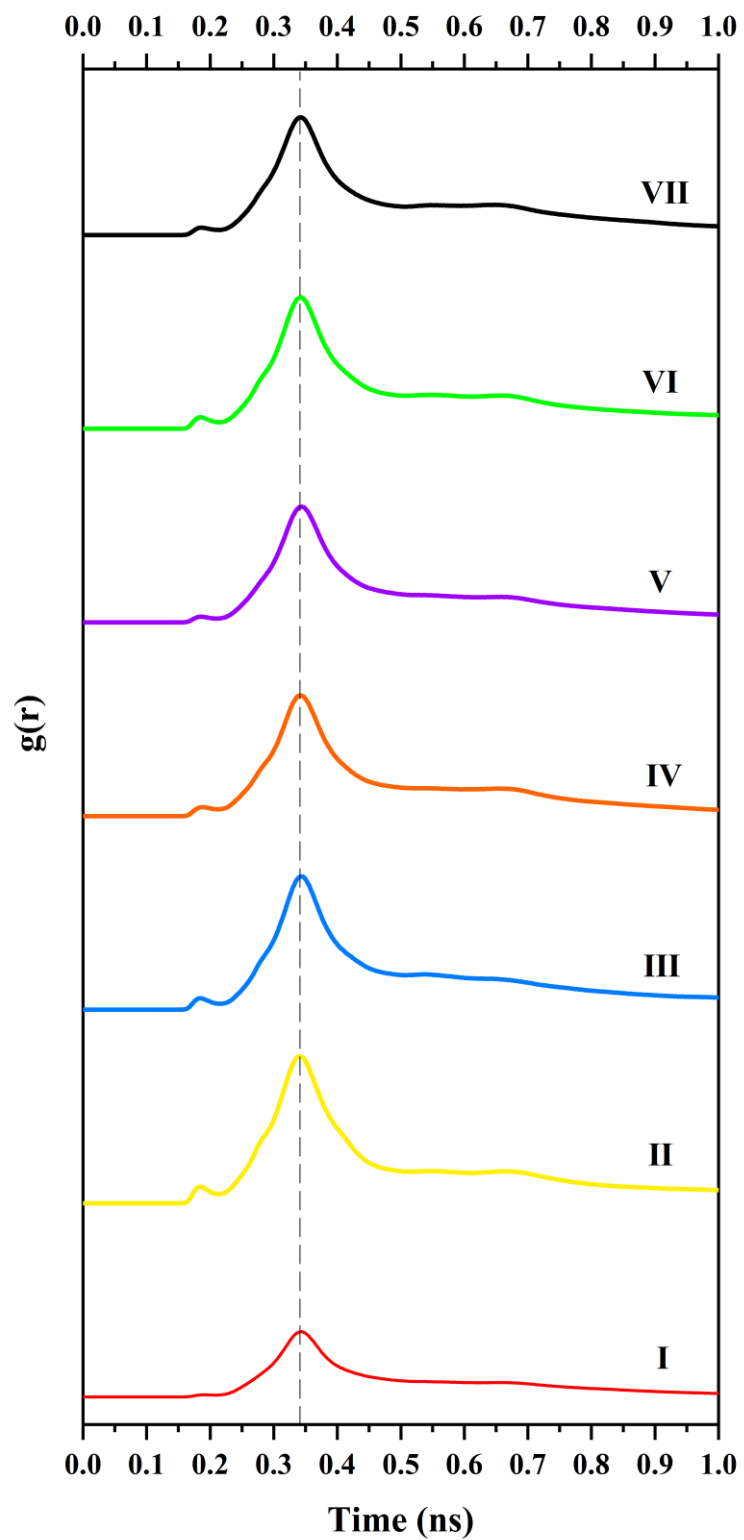


Figure S4. The RDFs between the dye anions based on the molecular surface in different systems

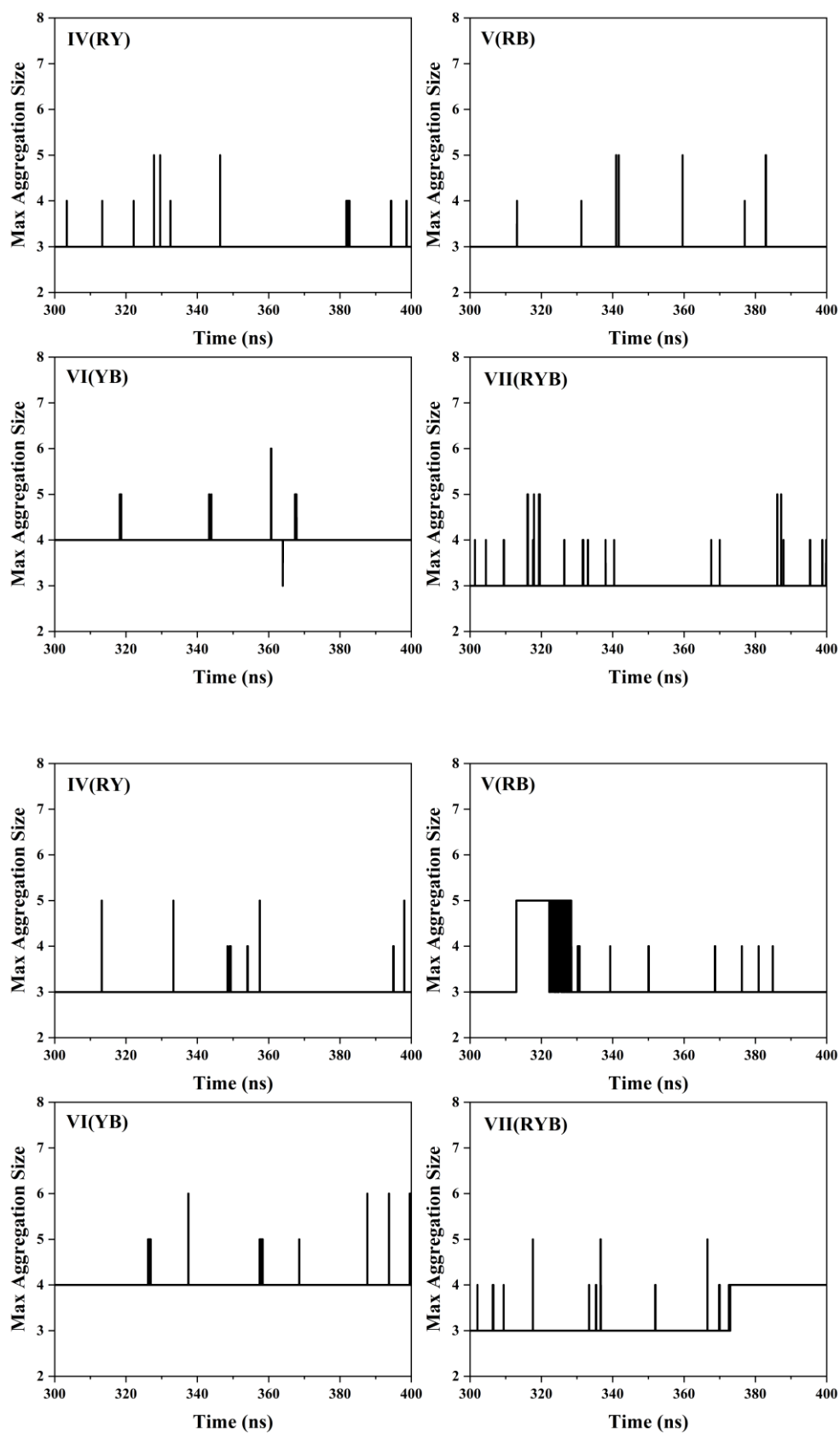


Figure S5. The max dye aggregation size of different dye mixture systems during 300 ~ 400 ns (for repeated simulations)