

Supporting Information

Remarkable static and dynamic nonlinear optical responses of Al₁₃-TCNQ/F4-TCNQ complexes: A quantum chemical study

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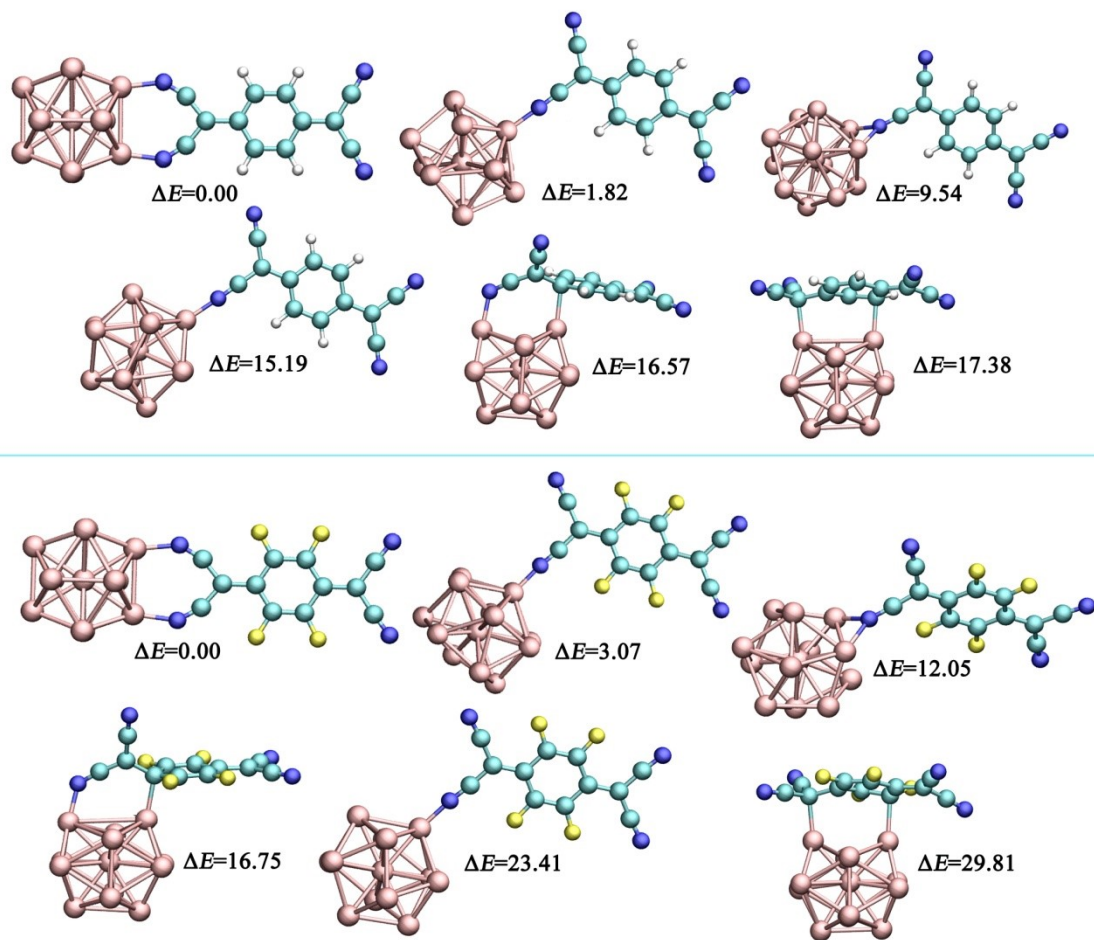


Fig. S1 Equilibrium structures with relative energy (in kcal mol⁻¹) of the Al₁₃-TCNQ and Al₁₃-F4-TCNQ at the PBE0/6-311G(d) level.

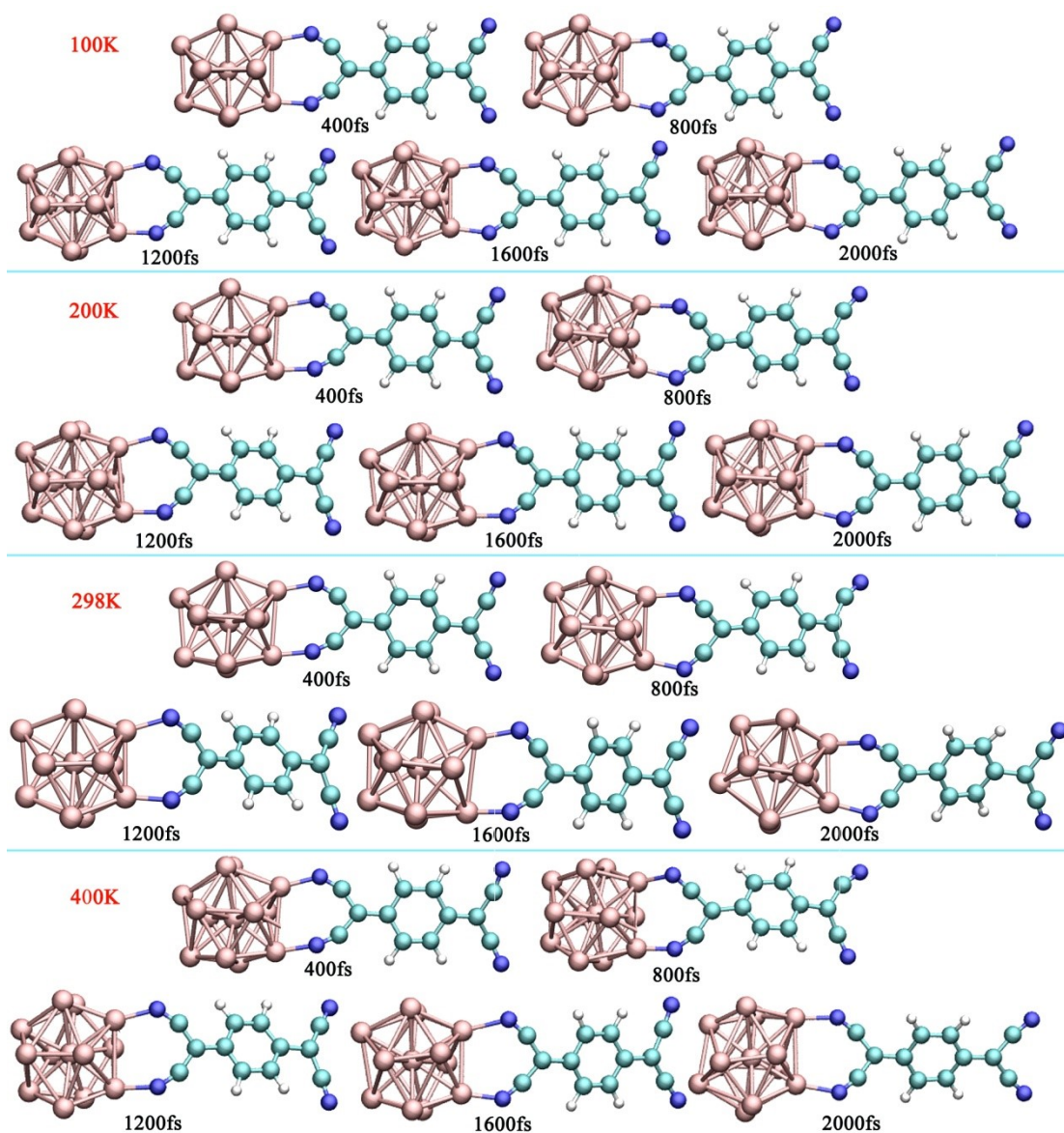


Fig. S2 Structures of Al₁₃-TCNQ at different time intervals during simulations at different temperatures.

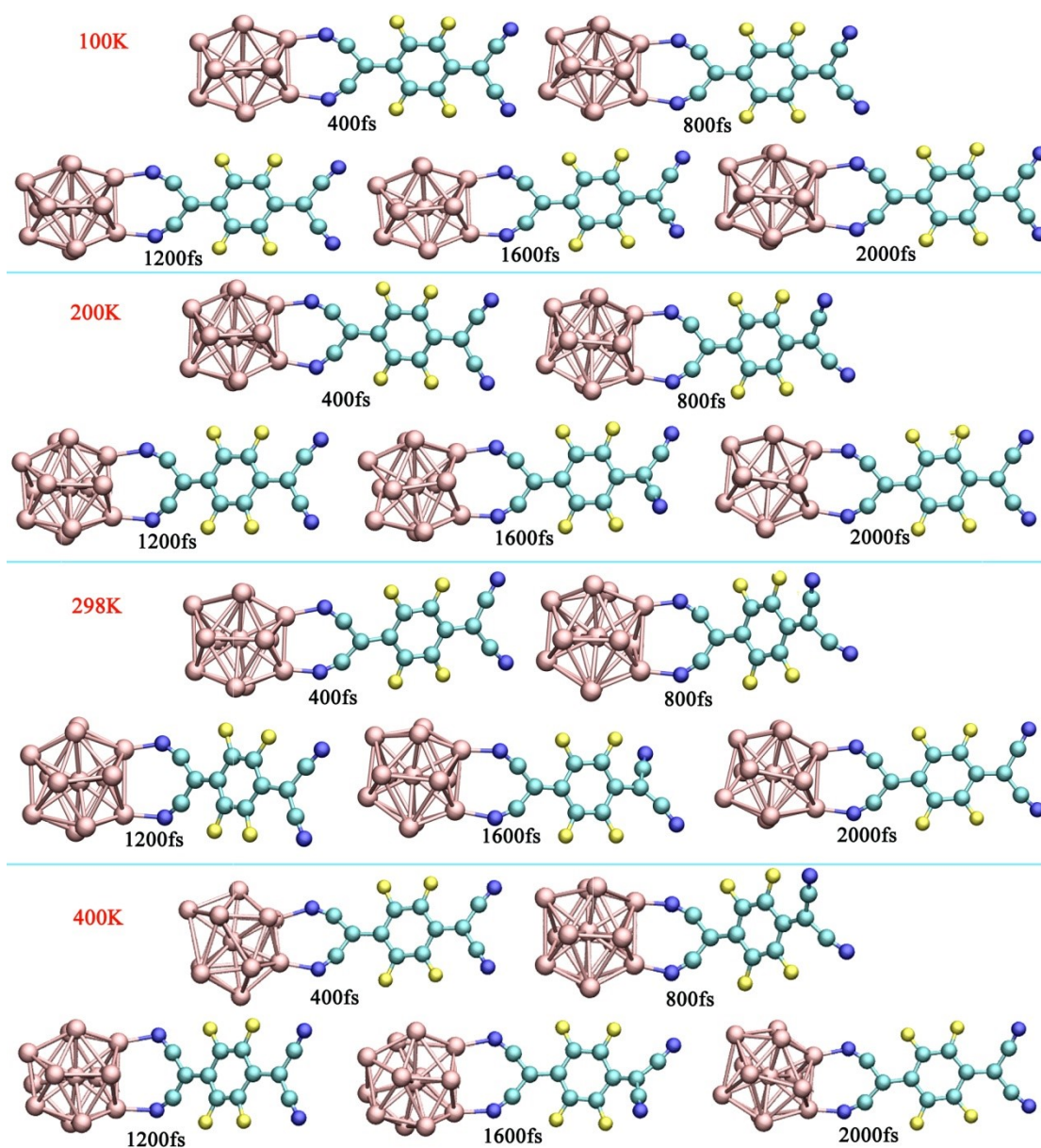


Fig. S3 Structures of Al₁₃-F4-TCNQ at different time intervals during simulations at different temperatures.