Theoretical Studies of the Additives for Copper Electroplating in PCB by DFT and MD simulation

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Table S1 HOMO and LUMO data of four kinds of leveling agent molecules

leveling agent	E_{HOMO}(eV)	E_{LUMO}(eV)	ΔE(eV)
DB	-5.723	0.595	6.318
Indigo	-5.298	-4.498	0.800
NTBC	-6.112	-3.664	2.448
ST	-5.162	-1.783	3.379

Table S2 The HOMO and LUMO data of eight kinds of inhibitor molecules

Inhibitor	E_{HOMO}(eV)	E_{LUMO}(eV)	ΔE(eV)
DSI	-6.153	-2.216	3.937
EPE	-4.800	-1.825	2.975
PPG	-5.613	0.614	6.227
PEG	-6.236	0.472	6.708
PEG 2000	-5.744	0.481	6.225
PEG 4000	-5.826	-0.623	5.203
PEG 6000	-5.550	-2.112	3.438
PEG 8000	-4.384	-4.312	0.072

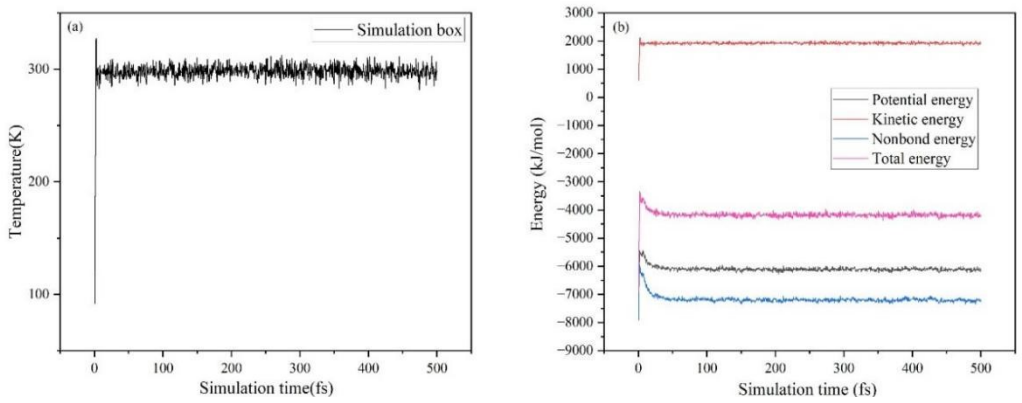

Fig. S1 The equilibrium of temperature (a) and energy (b) of DB

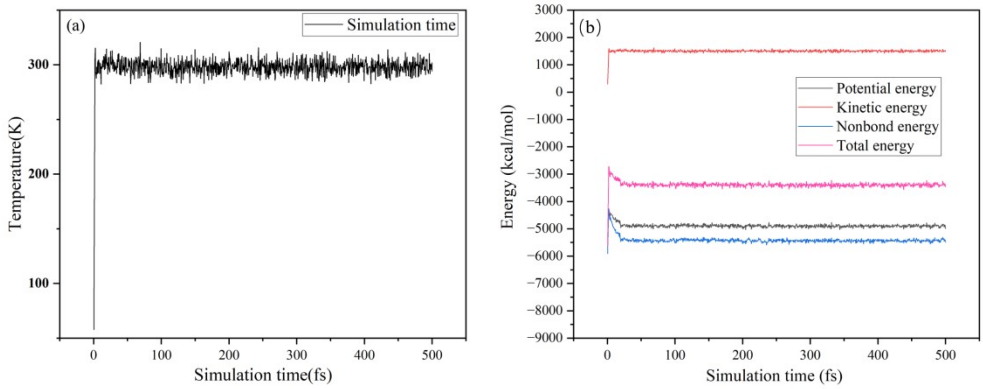

Fig. S2 The equilibrium of temperature (a) and energy (b) of Indigo

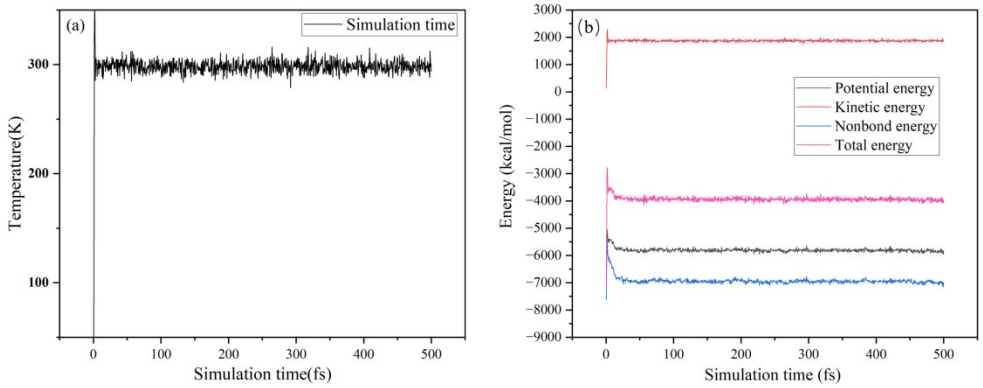

Fig. S3 The equilibrium of temperature (a) and energy (b) of NTBC

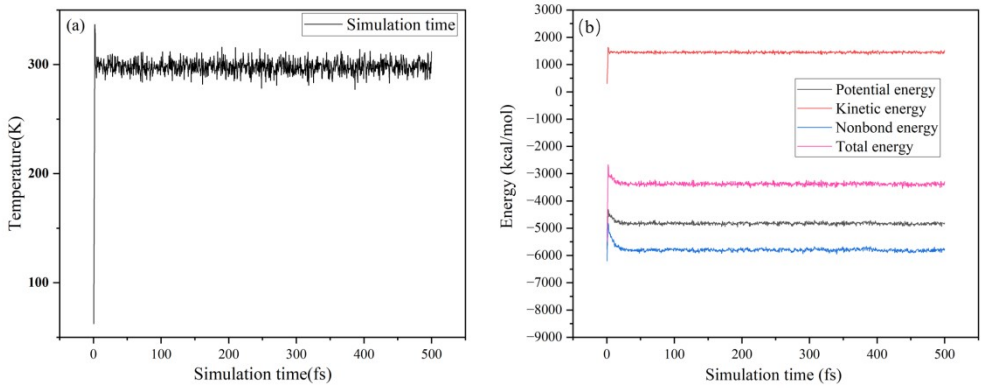

Fig. S4 The equilibrium of temperature (a) and energy (b) of ST

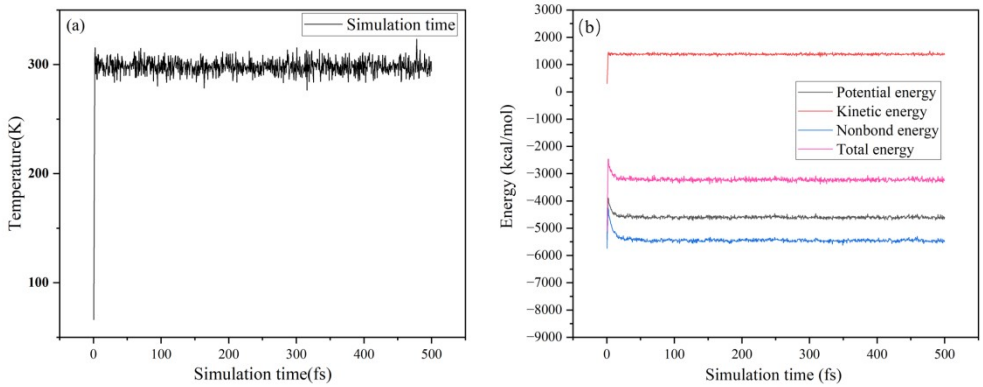

Fig. S5 The equilibrium of temperature (a) and energy (b) of DSI

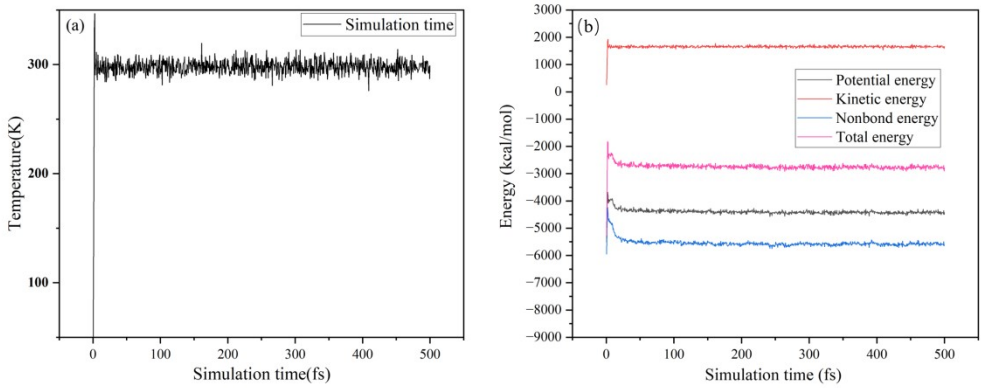

Fig. S6 The equilibrium of temperature (a) and energy (b) of EPE

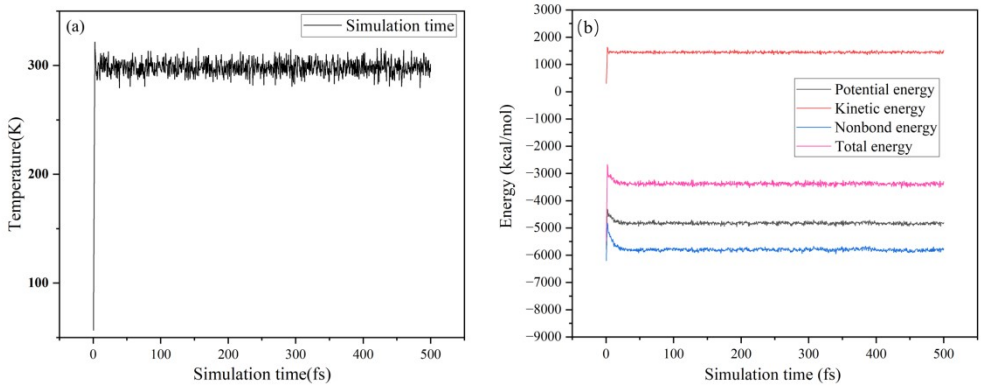

Fig. S7 The equilibrium of temperature (a) and energy (b) of PPG

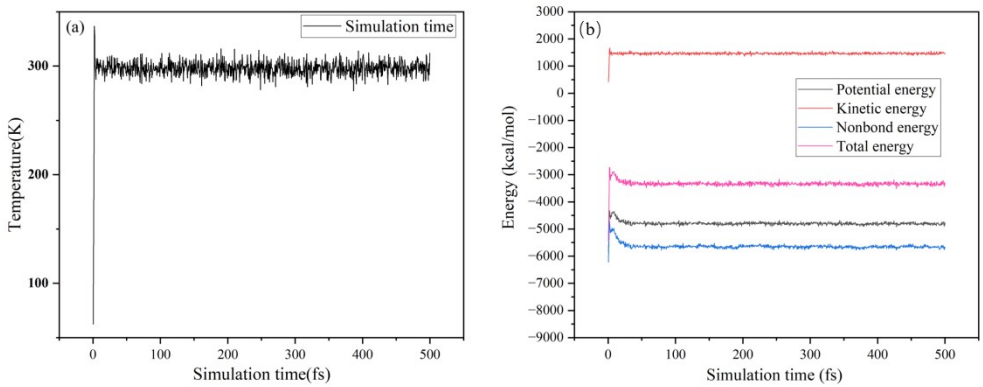

Fig. S8 The equilibrium of temperature (a) and energy (b) of PEG

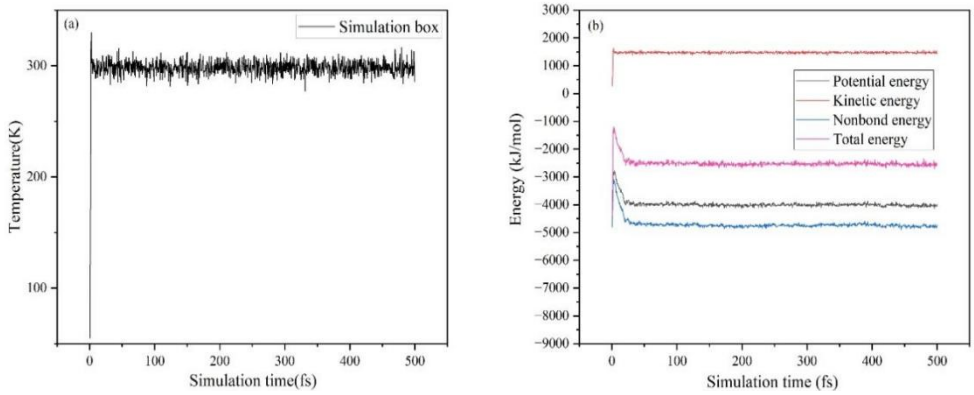

Fig. S9 The equilibrium of temperature (a) and energy (b) of PEG 2000

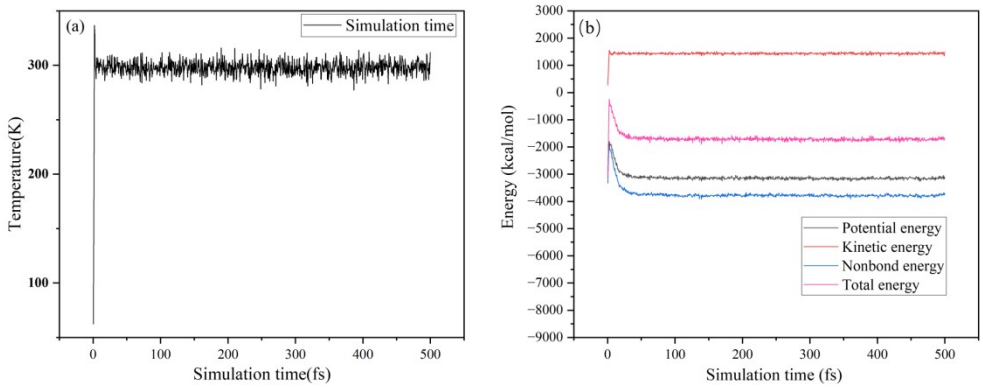

Fig. S10 The equilibrium of temperature (a) and energy (b) of PEG 4000

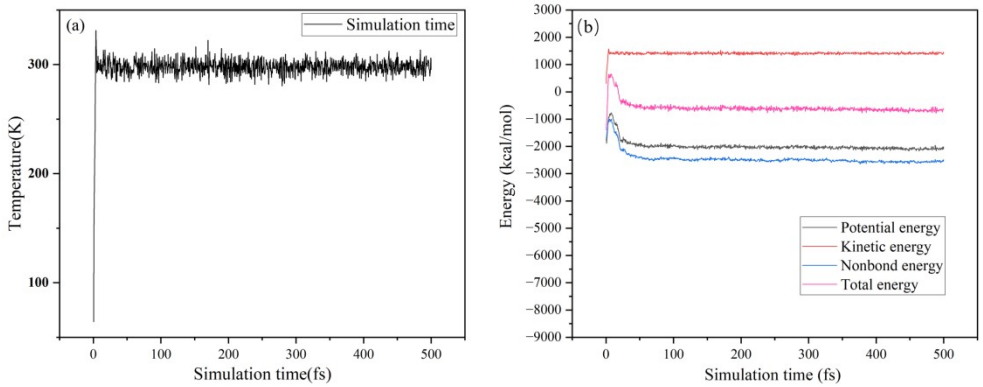

Fig. S11 The equilibrium of temperature (a) and energy (b) of PEG 6000

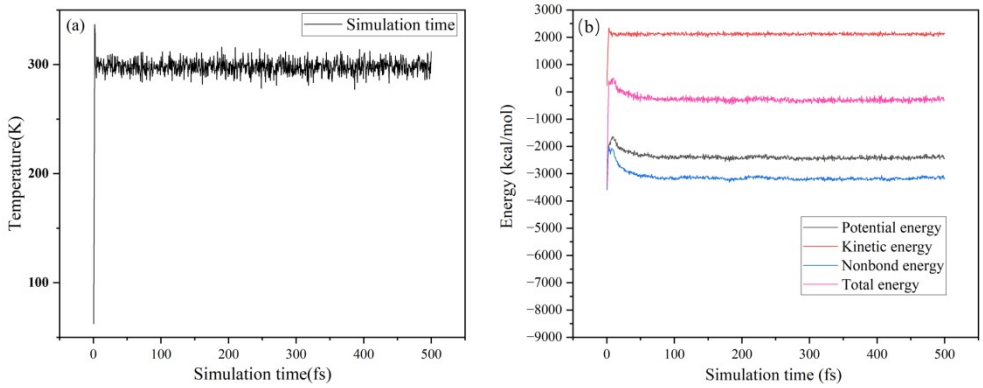

Fig. S12 The equilibrium of temperature (a) and energy (b) of PEG 8000