Electronic Supplementary Information (ESI) Available

ReaxFF Reactive Molecular Dynamics on Silicon Pentaerythritol Tetranitrate Crystal Validates the Mechanism for the Colossal Sensitivity

(Tingting Zhou, Lianchi Liu, William A. Goddard III, Sergey V. Zybin, Fenglei Huang)

Table S1 Bond-order cutoffs for various atom pairs used in the algorithm of molecule recognition

	C	H	O	N	Si
C	0.55	0.40	0.60	0.30	0.40
H		0.55	0.40	0.55	0.40
O			0.65	0.40	0.55
N				0.55	0.40
Si					0.55

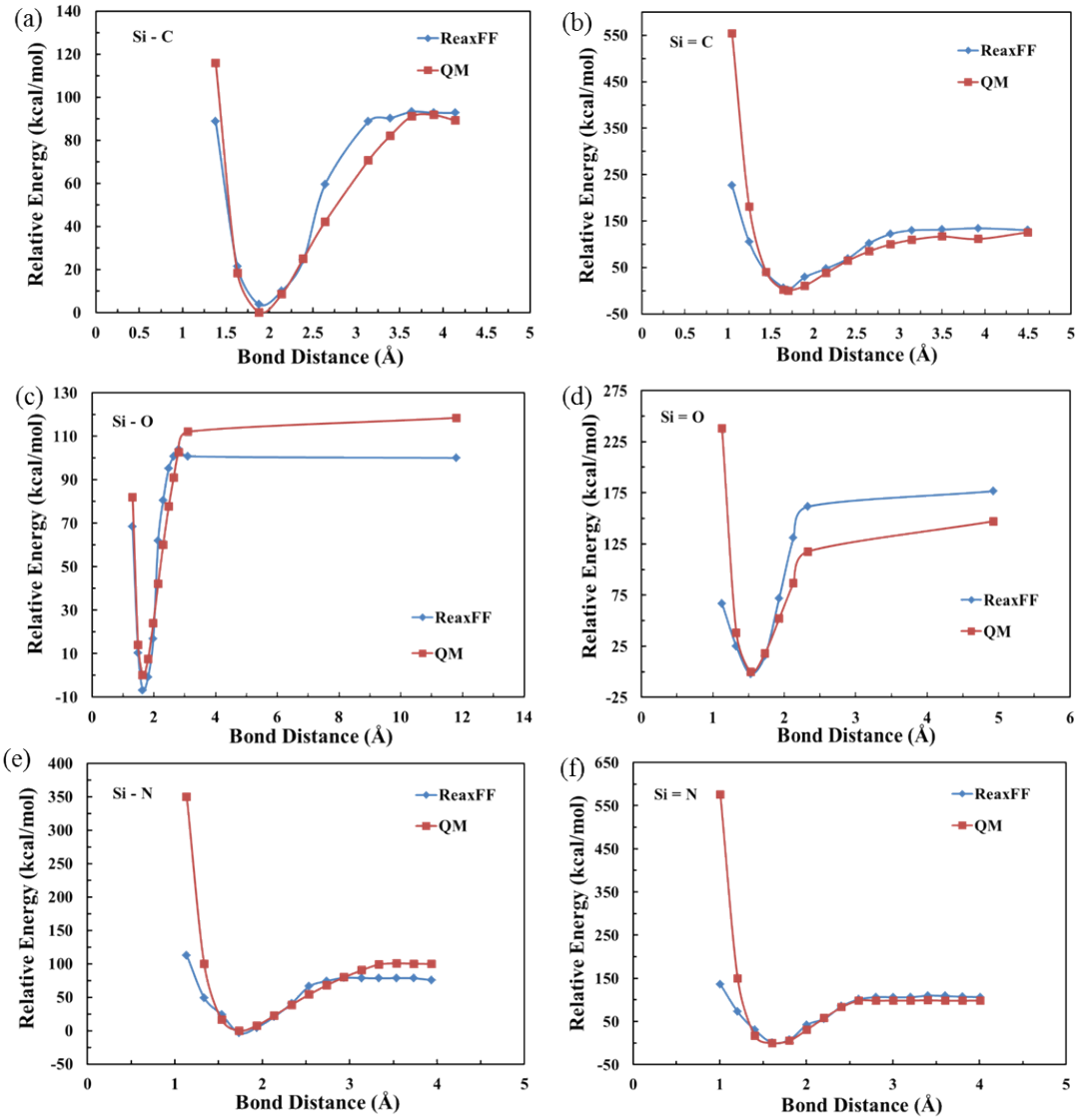

Figure S1. Comparisons of ReaxFF and QM energies for Si—C (a-b), Si—O (c-d), and Si—N (e-f) bond dissociations.

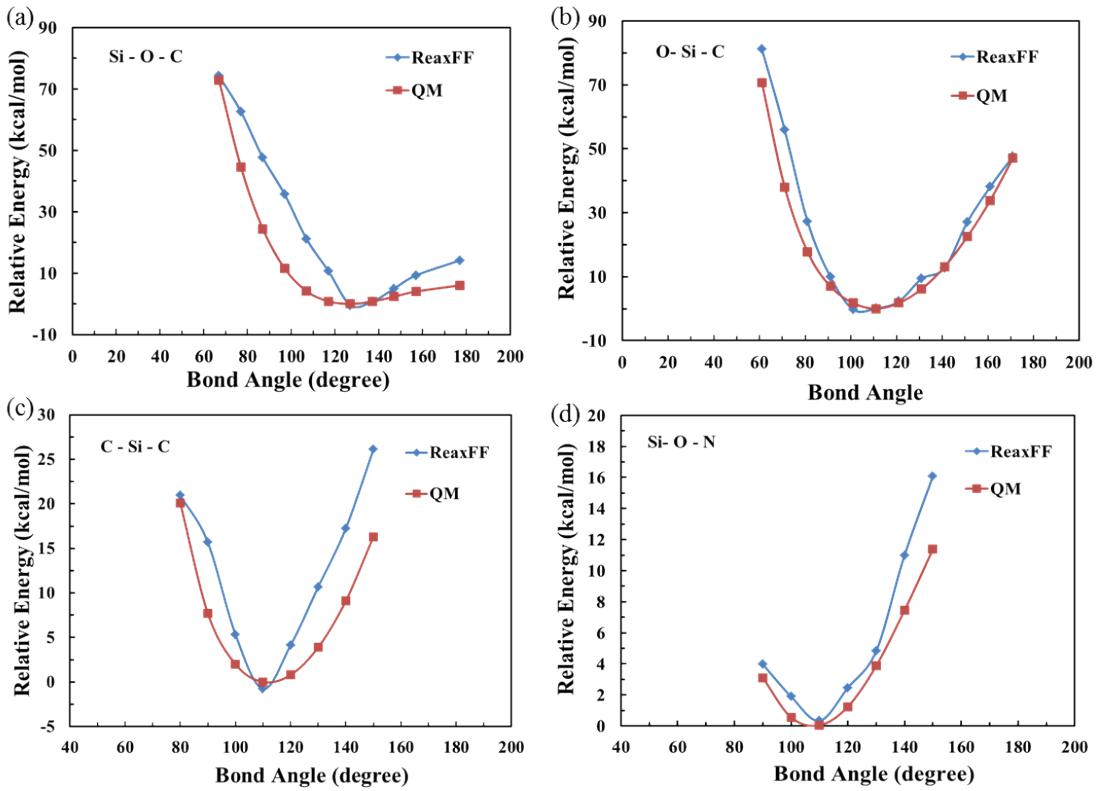

Figure S2. Comparisons of ReaxFF and QM bending energies for Si—O—C (a), O—Si—C (b), C—Si—C (c), and Si—O—N (d) angles.