Supporting Information

Oxygen Balance Leads to Enhanced Performance in Environmentally Acceptable High-Energy Density Materials: Predictions from First-Principles Molecular Dynamics Simulations

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Table S1. Bond order cut-off values for different atom pairs.

	C	H	O	N	Si
C	0.55	0.40	0.80	0.30	0.30
H		0.55	0.40	0.55	0.30
O			0.65	0.55	0.30
N				0.45	0.30

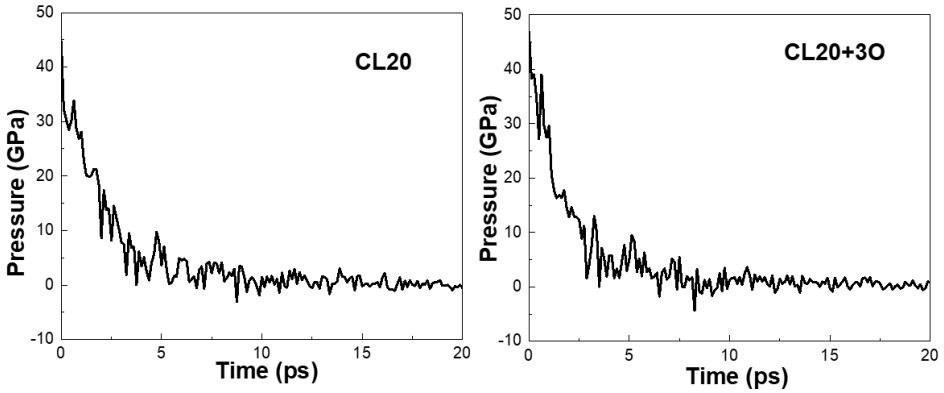

Figure S1. Evolution of the system pressure during constant temperature simulation of 8 times volume expansion over 20 ps.