Prediction of the Chapman-Jouguet Chemical Equilibrium State in a Detonation Wave from First Principles Based Reactive Molecular Dynamics

Supporting Information:

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1. Time evolution of Hugoniot function and potential energy of RDX system

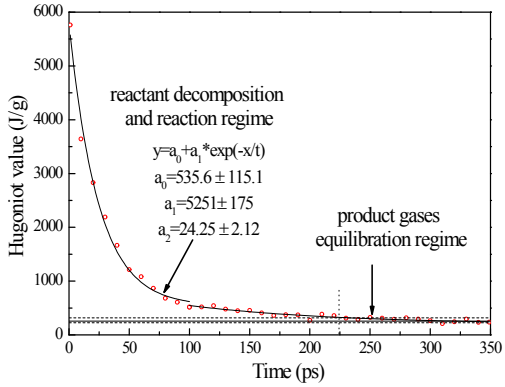

Fig.S1. Time evolution of the Hugoniot function for RDX at T=2700 K and V/V0=0.85. The solid horizontal line shows an average over the final 100 ps of simulation while the dashed lines mark the standard deviation above and below the average values from five independent simulations.

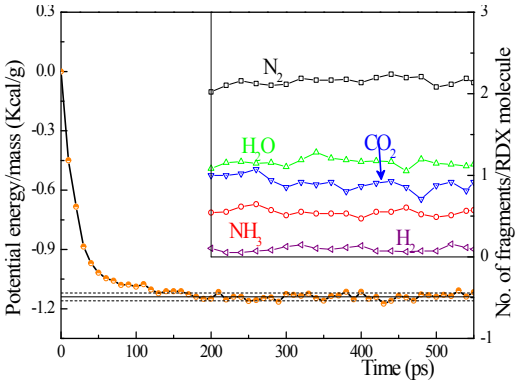

Fig.S2. Time evolution of potential energy per unit mass and reaction products (insert for 200 ps to 550 ps of NVT simulation) for RDX at T=2690 K and V/V0=0.76. The solid horizontal line shows an average over the final 100 ps of simulation while the dashed lines mark the standard deviation above and below the average values from five independent simulations.

2. The Time evolution of Hugoniot function and potential energy, as well as family of Isotherms and Crussard Curve of PETN, HMX and H_2/O_2 system

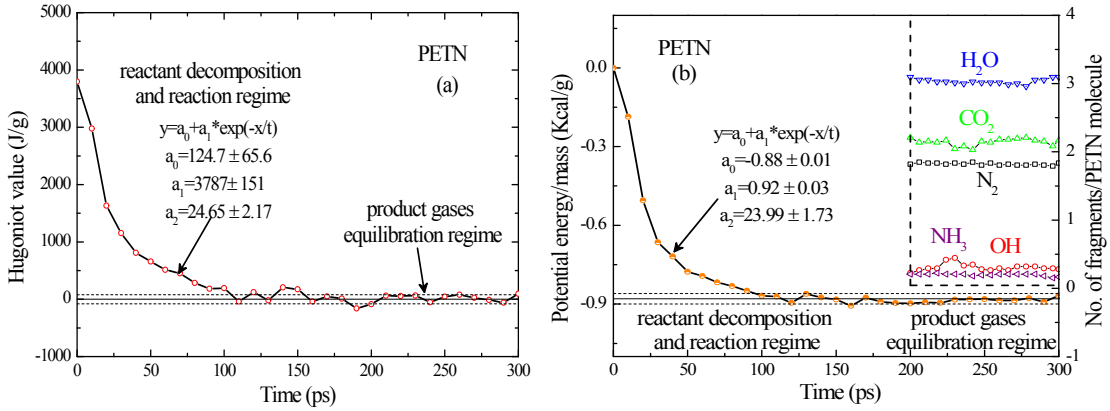

Fig. S3. Time evolution of (a) the Hugoniot function (b) the potential energy per unit mass and reaction products (insert for the last 100ps of NVT simulation) in for PETN at T=2500 K and V/V0=0.85. The solid horizontal line shows an average over the final 100 ps of simulation, and while the dashed lines mark the standard deviation above and below the average values from five independent simulations.

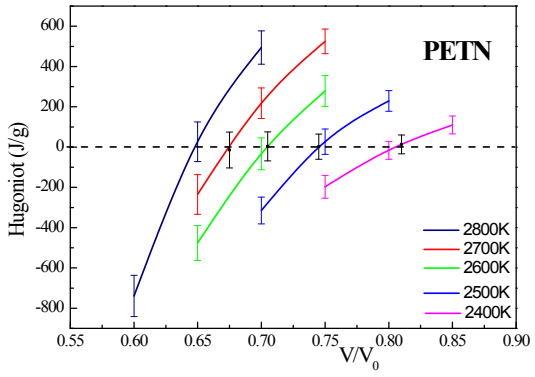

Fig. S4. The family of isotherms (spline fitted) for PETN at compression ratios from 0.60 to 0.85 for five different temperatures. This provides five points along the Crussard isentrope: V/V_0=0.650 at 2800 K, 0.675 at 2700 K, 0.705 at 2600 K, 0.735 at 2500 K, and 0.810 at 2400 K.

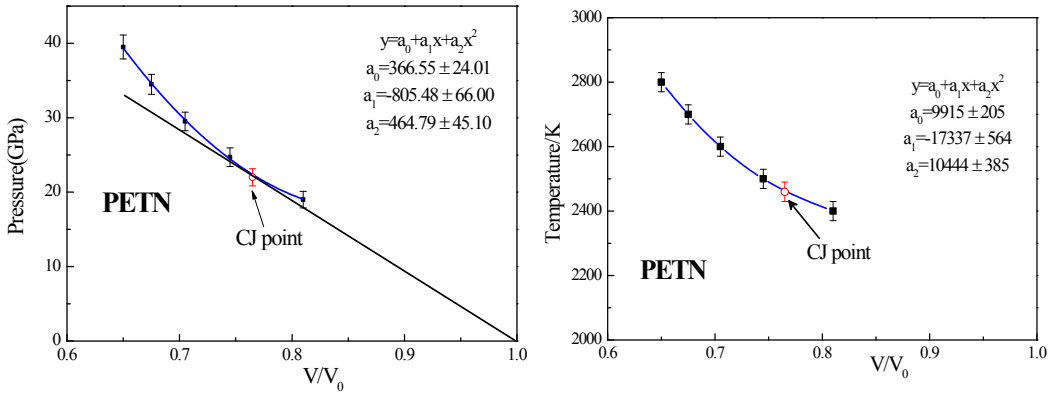

Fig. S5. (Left) Calculation of the CJ point parameters for PETN: compression ratio V/V_0=0.765 and pressure P_{CJ} = 22.47 GPa. (Right) Equilibrium temperatures for the various points along the Crussard curve, fitted to a quadratic polynomial. The predicted CJ temperature is 2460 K, as indicated by the circle.

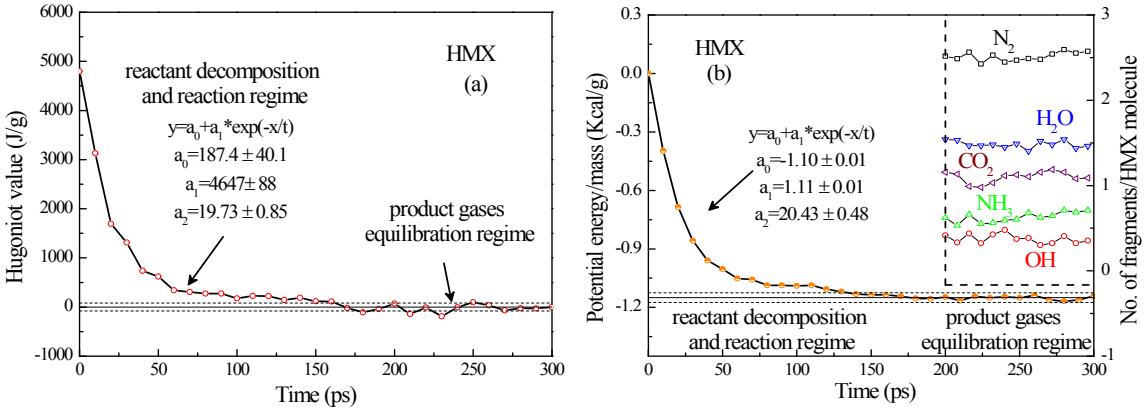

Fig. S6. Time evolution of (a) the Hugoniot function (b) the potential energy per unit mass and reaction products (insert for the last 100ps of NVT simulation) in for HMX at T=2600 K and V/V0=0.8. The solid horizontal line shows an average over the final 100 ps of simulation, and while the dashed lines mark the standard deviation above and below the average values from five independent simulations.

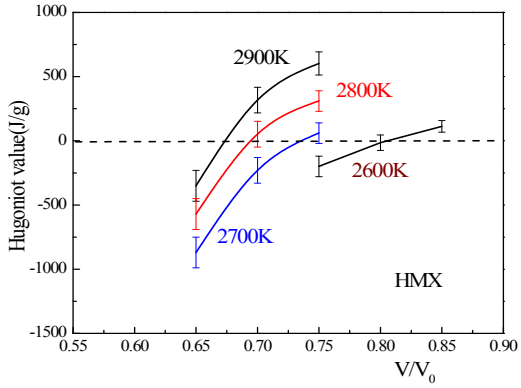

Fig. S7. The family of isotherms (spline fitted) for HMX at compression ratios from 0.65 to 0.85 for four different temperatures. This provides four points along the Crussard isentrope: V/V_0=0.67 at 2900 K, 0.695 at 2800 K, 0.735 at 2700 K and 0.805 at 2600 K.

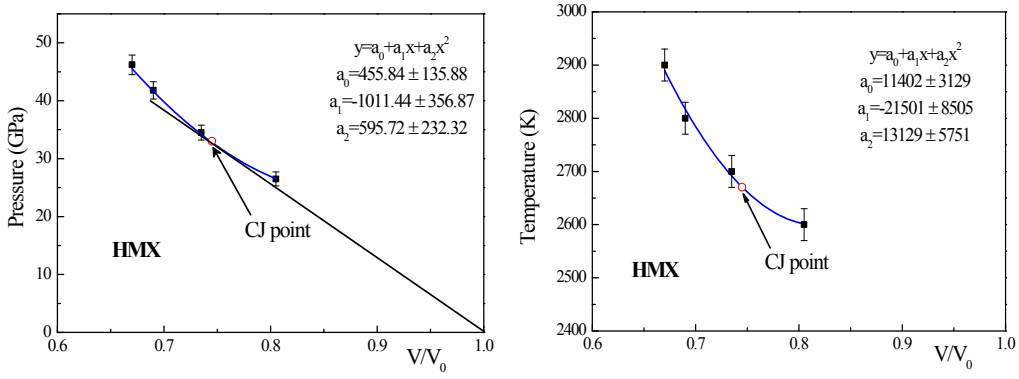

Fig. S8. (Left) Calculation of the CJ point parameters for HMX: compression ratio V/V_0=0.75 and pressure P_{CJ} = 32.68 GPa. (Right) Equilibrium temperatures for the various points along the Crussard curve, fitted to a quadratic polynomial. The predicted CJ temperature is 2680 K, as indicated by the circle.

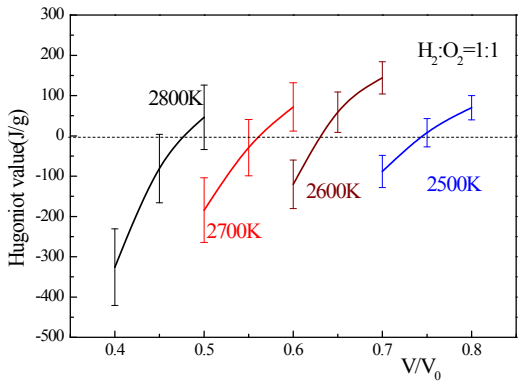

Fig. S9. The family of isotherms (spline fitted) for H_2/O_2 at compression ratios from 0.40 to 0.8 for four different temperatures. This provides four points along the Crussard isentrope: V/V_0=0.49 at 2800 K, 0.56 at 2700 K, 0.63 at 2600 K, 0.740 at 2500 K.

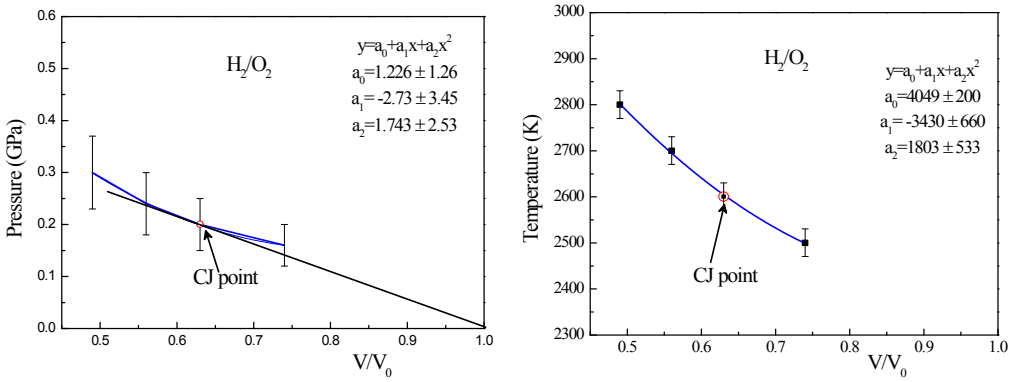

Fig. S10. (Left) Calculation of the CJ point parameters for H_2/O_2 mixture: compression ratio V/V_0=0.63 and pressure P_{CJ} = 0.198 GPa. (Right) Equilibrium temperatures for the various points along the Crussard curve, fitted to a quadratic polynomial. The predicted CJ temperature is 2600 K, as indicated by the circle.

Table S1. Detonation Products predicted at the CJ state of H_2/O_2

		H_2/O_2
		ReaxFF
Density(g/cm^3)		0.09
D_{CJ}(m/s)		2538±377
Products(mol/mol)	H_2O	0.927
	O_2	0.459
	H_2O_2	0.020
	HO_2	0.034
	HO	0.037
	H_2	0.008
	Material recovery(%)[a]	
	H	99
	O	99.5

a) the experimental detonation velocity is ranging from 2800 to 3000 m/s at the initial pressures up to 1 bar and densities up to 1-3 kg/m^3 .[25]

2. Bond Order Cut-Off Values

Table S2. Bond order cut-off values for different atom pairs. *BondFrag* program in the LAMMPS code uses these values as a default parameter set (can be adjusted by the user) to determine molecular fragments (there is no connection if the calculated bond order is less than cut-off value).

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