

Supporting Information

Effects of noncovalent interactions on the impact sensitivity of HNS-based cocrystals:

A DFT study

Xiao Zhao, Shiliang Huang, Yu Liu, Jinshan Li, Weihua Zhu*

Table S1. Crystal parameters and impact sensitivity of pure HNS crystal and HNS/BP, HNS/BPE, HNS/BPA cocrystals.

	HNS		HNS/BP		HNS/BPE		HNS/BP A	
	expt.	cal.	expt.	cal.	expt.	cal.	expt.	cal.
a/Å	22.3260	22.0548	30.2383	28.9091	31.5882	30.4085	31.8694	30.8972
b/Å	5.57060	5.61963	5.5203	5.63118	5.8953	6.04125	5.8964	6.01383
c/Å	14.6670	14.8559	14.8056	14.9195	14.4728	14.3711	14.5682	14.6530
α /°	90.00	90.00	90.00	90.00	90.00	90.00	90.00	90.00
β /°	111.040	111.617	85.282	83.094	90.548	88.862	91.408	90.438
γ /°	90.00	90.00	90.00	90.00	90.00	90.00	90.00	90.00
V/ Å ³	1713.68	1711.75	2463.04	2411.15	2695.02	2639.53	2736.8	2722.60
ρ /g/cm ³	1.74508	1.74705	1.63535	1.67055	1.55875	1.59153	1.48977	1.49751
IS/cm	22		106.9		100.9		44.2	

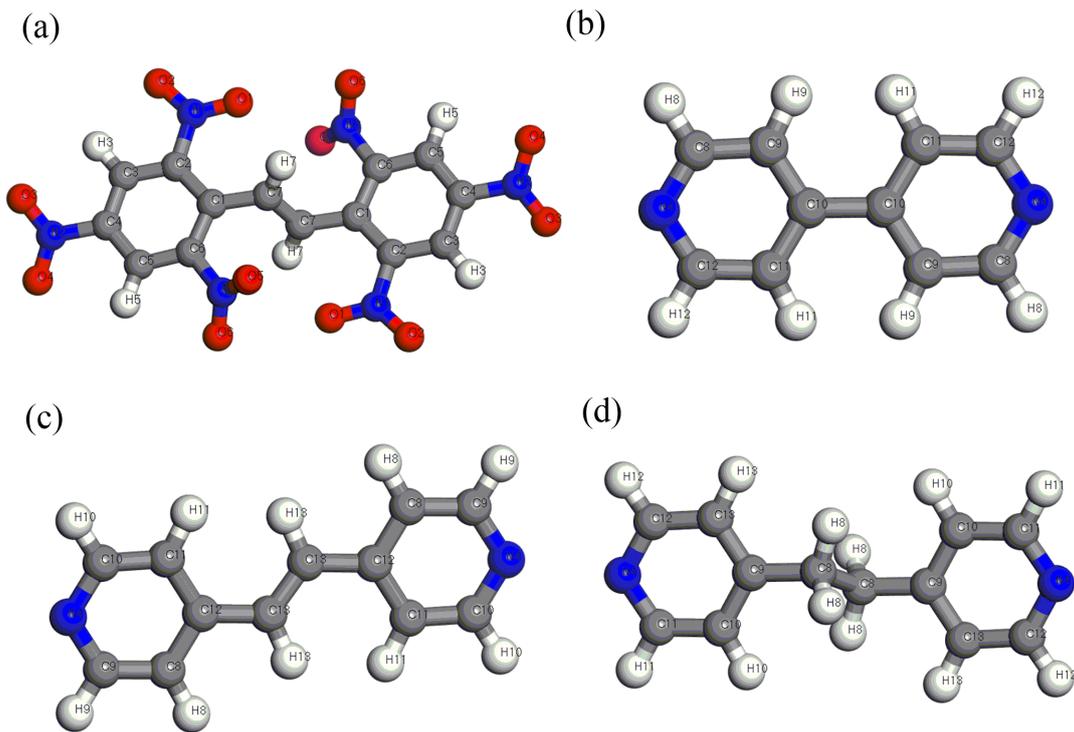


Figure S1. Geometrical configuration of components molecular.(a) for HNS, (b) for BP, (c) for BPE and (d) for BPA.

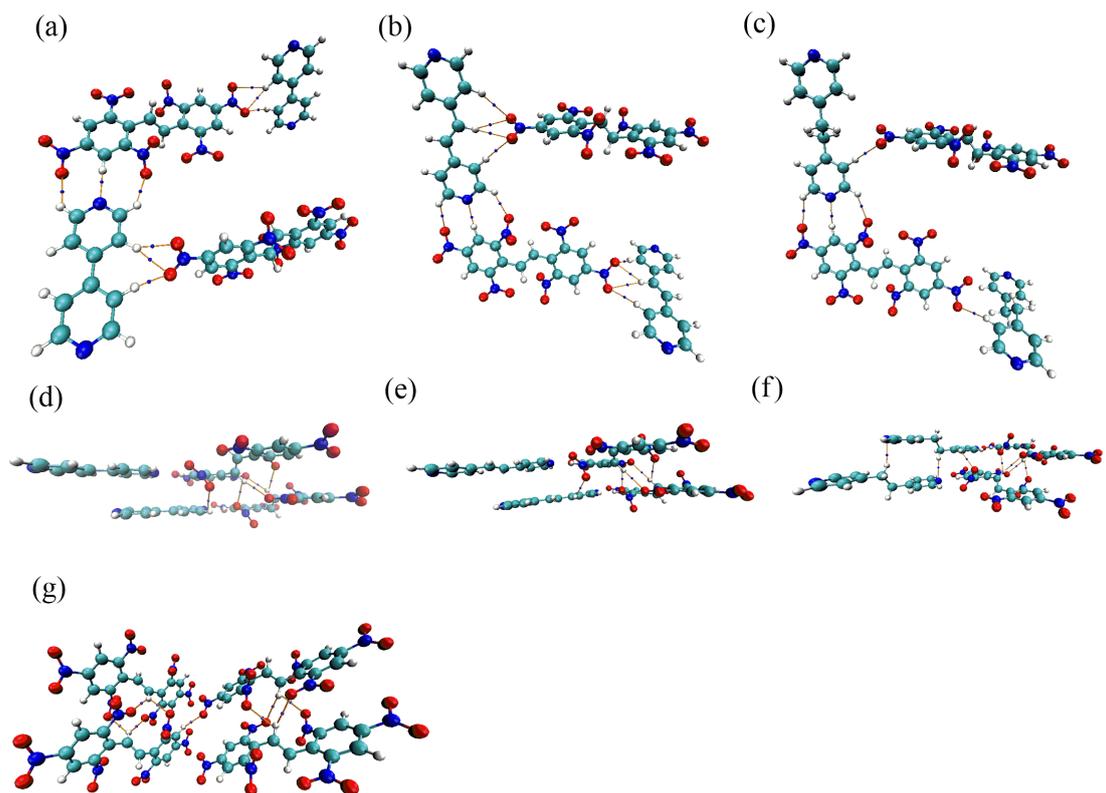


Figure S2. Detailed information for geometry structure, bond paths(represented by orange lines) and (3,-1) critical point(represented by blue spheres) in particular clusters: (a)BP intra, (b) BPE intra, (c) BPA intra, (d) BP inter, (e) BPE inter, (f) BPA inter and (g) HNS pure.

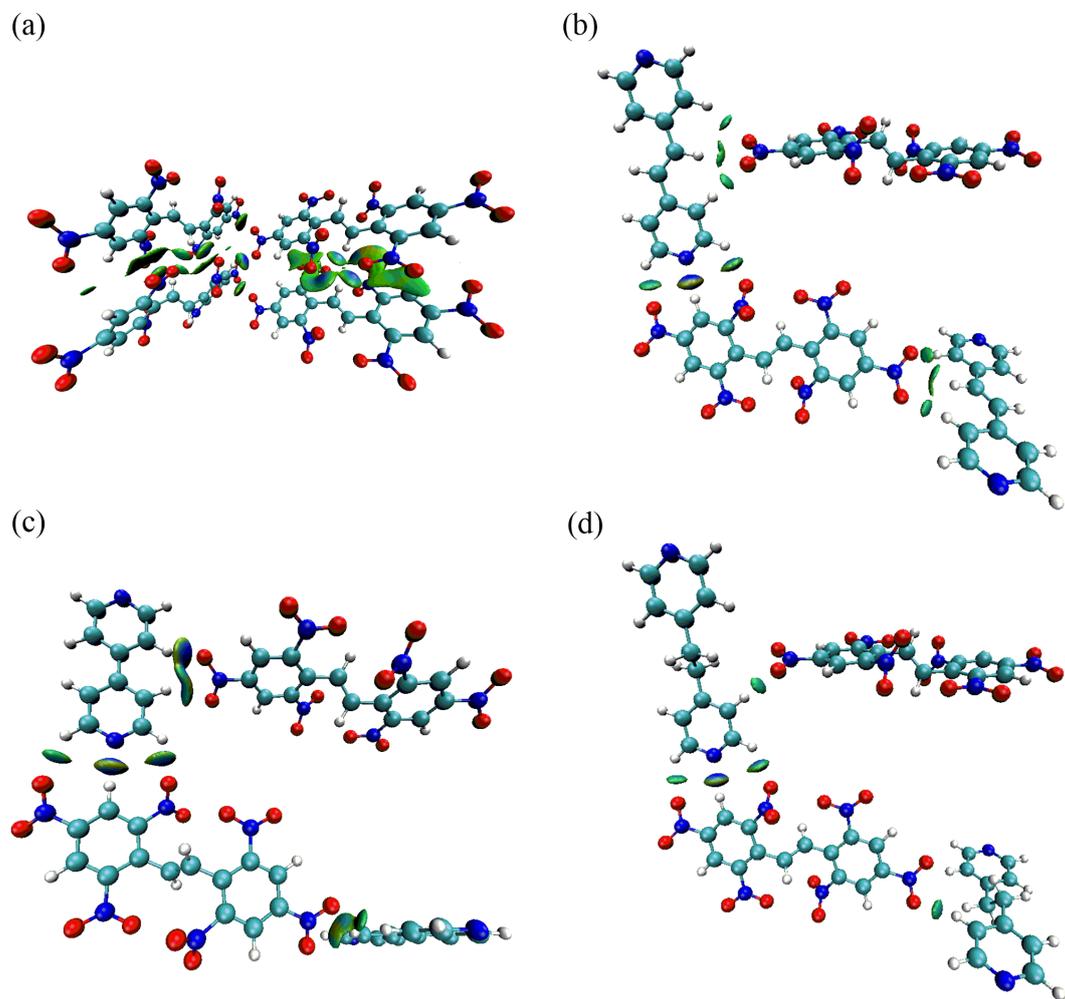


Figure S3. NCI plots for gradient isosurfaces(0.01 a.u.) for intralayer clusters: (a) HNS pure, (b) BP intra, (c) BPE intra and (d) BPA intra. The blue-green-red scale color on surfaces denotes strong attractive, weak attractive and nonbonded interaction respectively.