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Research paper

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Relaxed structure of typical nitro explosives in the excited state:

Observation, implication and application

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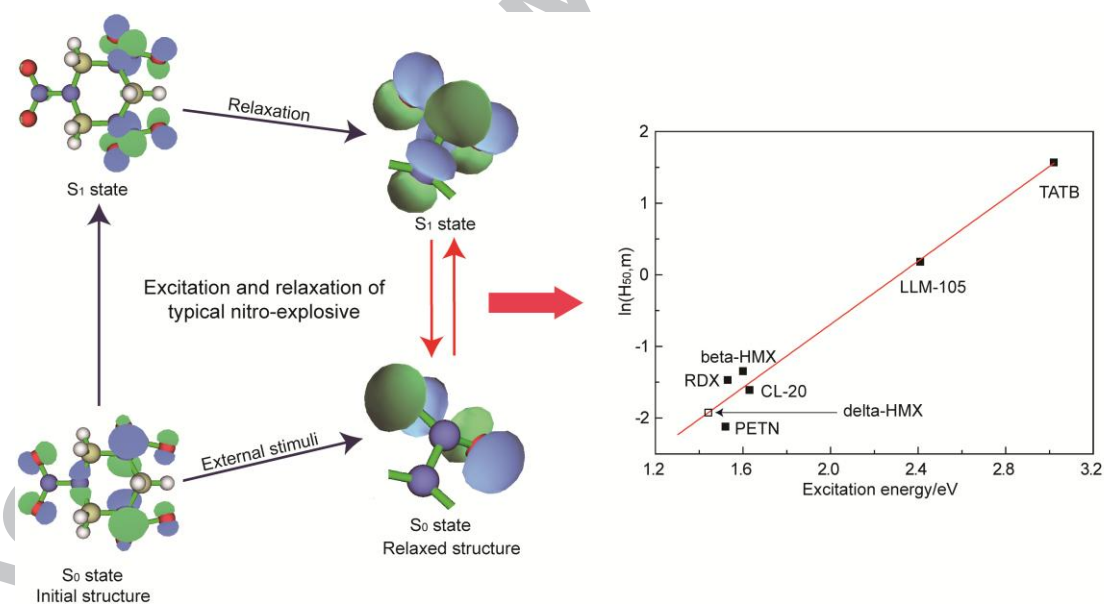
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Graphical abstract



Highlights

Relaxed structures of nitro explosives in the excited state are investigated.

Typical nitro explosives exhibit a similar relaxation behavior.

Impact sensitivity is related to excitation energy of relaxed structure.

High sensitivity δ -HMX has a lower excitation energy for relaxed structure than β -HMX

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