CL-20 is powerful energetic material with good detonation performance, but high sensitivity limits its widespread implementation. Nitroguanidine (NQ) is proposed as a cocrystal to limit the sensitivity of CL-20. Molecular Dynamics simulations and Density Functional Theory are used to optimize the molecular ratio and intermolecular interaction nature of the CL-20/NQ cocrystal explosive. By increasing the strength of trigger bonds van der Waals forces reduce the sensitivity of the cocrystal explosive.

GRAPHICAL ABSTRACT FIGURE:

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