

New insight into the structural evolution of PbTiO₃: An unbiased structure search

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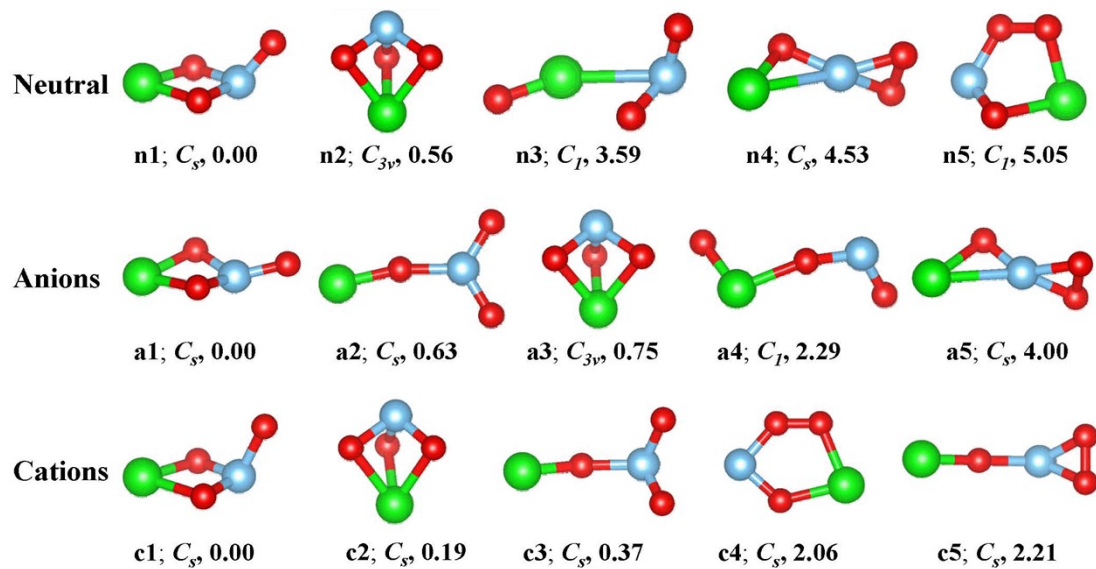


Figure S1. The metastable structures of neutral and charged PbTiO_3 clusters, together with symmetry and relative energy corresponding to the ground state structures.

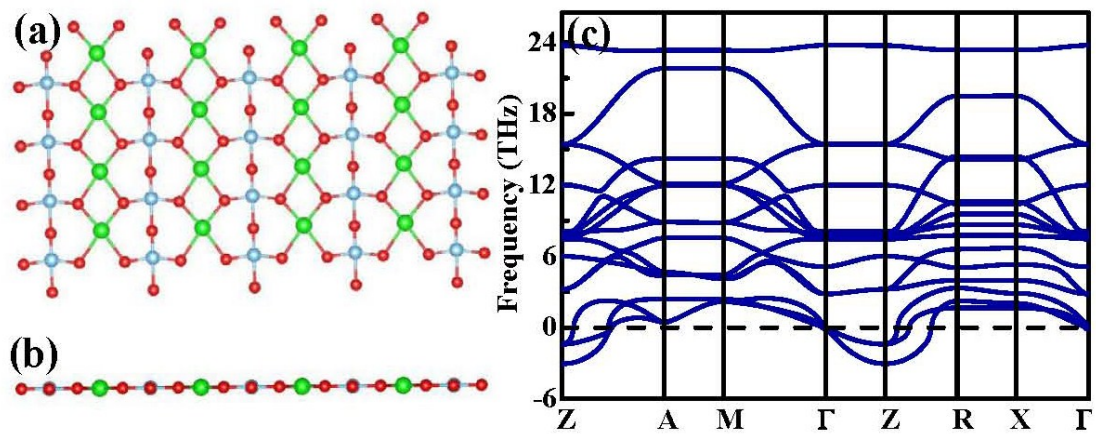


Figure S2. The ball and stick model (Top (a) and side (b) views), phonon dispersion relations (c) of the lowest energy two-dimensional (2D) monolayer PbTiO₃.