materials

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*Supporting information*

# Excellent Infrared Nonlinear Optical Crystals $BaMO(IO_3)_5$(M = V, Ta) Predicted by First Principle Calculations

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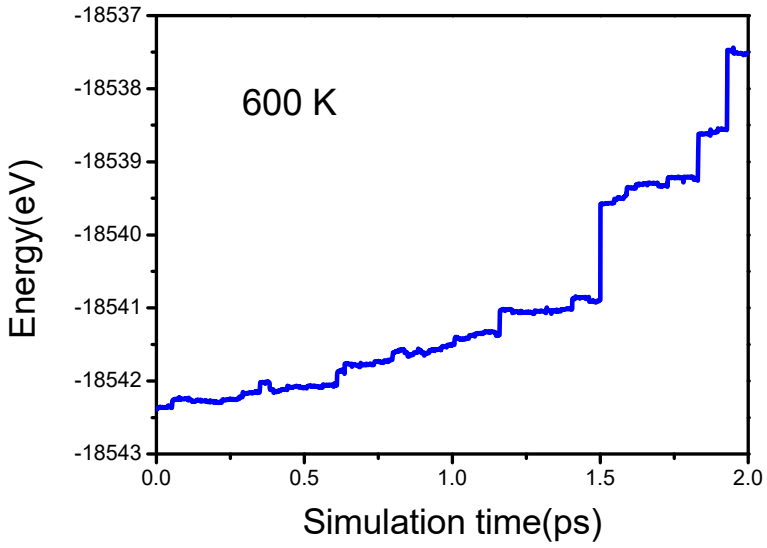


**Figure S1.** The energy evolution curves of the $BaTaO(IO_3)_5$ at 600 K during the dynamics simulation.

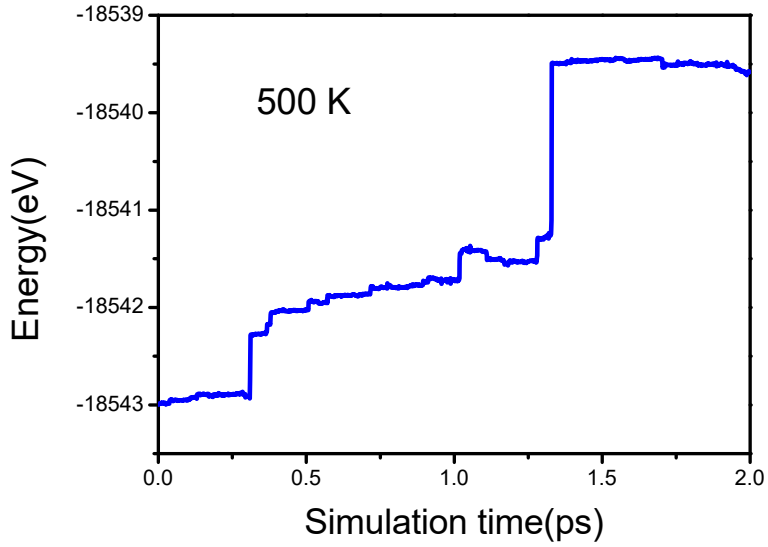


**Figure S2.** The energy evolution curves of the $BaTaO(IO_3)_5$ at 500 K during the dynamics simulation.