

First-Principles Study on Strain-Engineered Photocatalytic Performance in Ferroelectric $\text{K}(\text{Ta}_{0.5}\text{Nb}_{0.5})\text{O}_3$

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Strain/Pa	-5 (PBE)	0 (PBE)	5 (PBE)	-5 (HSE06)	0 (HSE06)	5 (HSE06)
band gap/eV	1.915	2.21	1.83	3.34	4.05	3.60

Table A1. The crystal system of KTN under different strain effects.