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Supporting information for article:

***R*-3c-type half-metals of LnNiO₃ (Ln = La, Ce, Nd, Pm, Gd, Tb, Dy, Ho, Er, Lu) with multiple dirac cones: a potential class of advanced spintronic materials**

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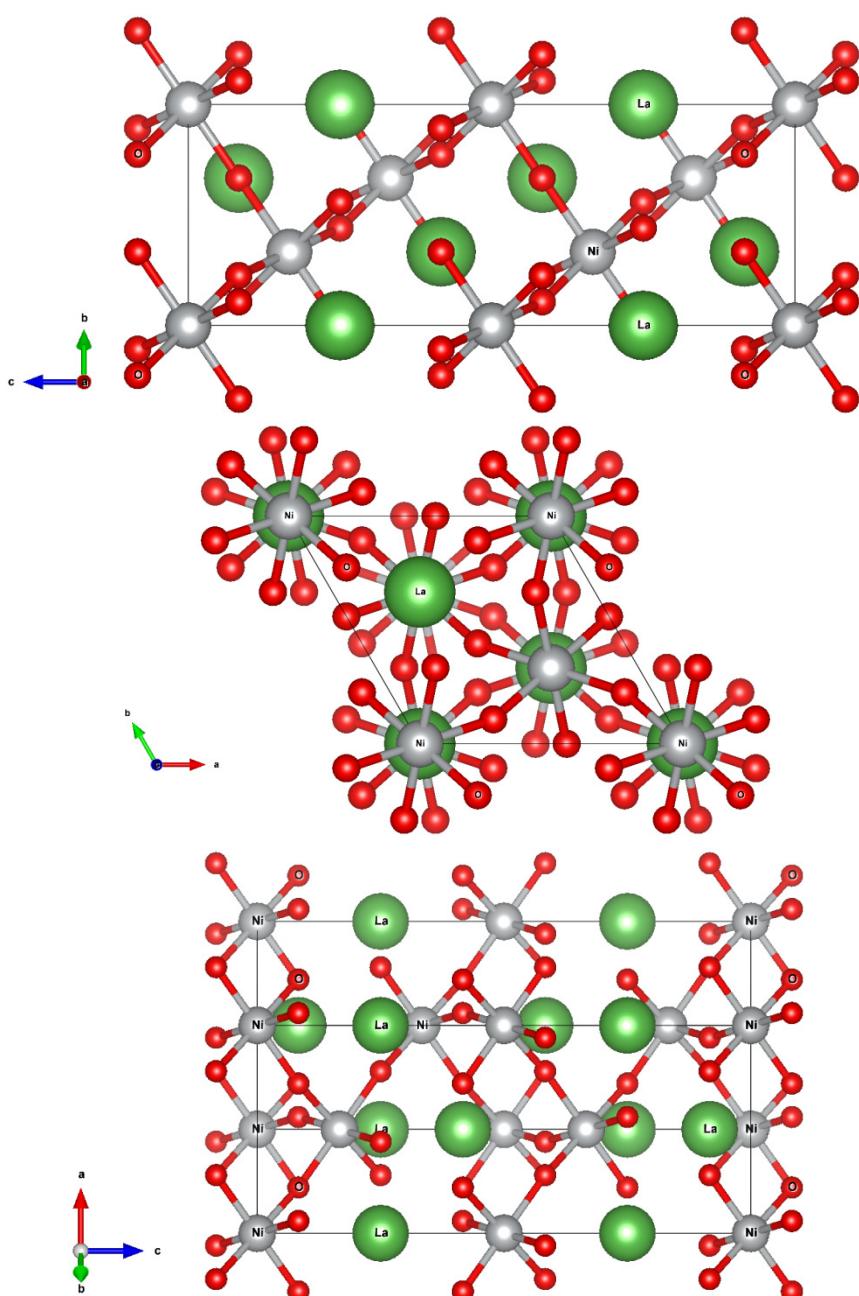
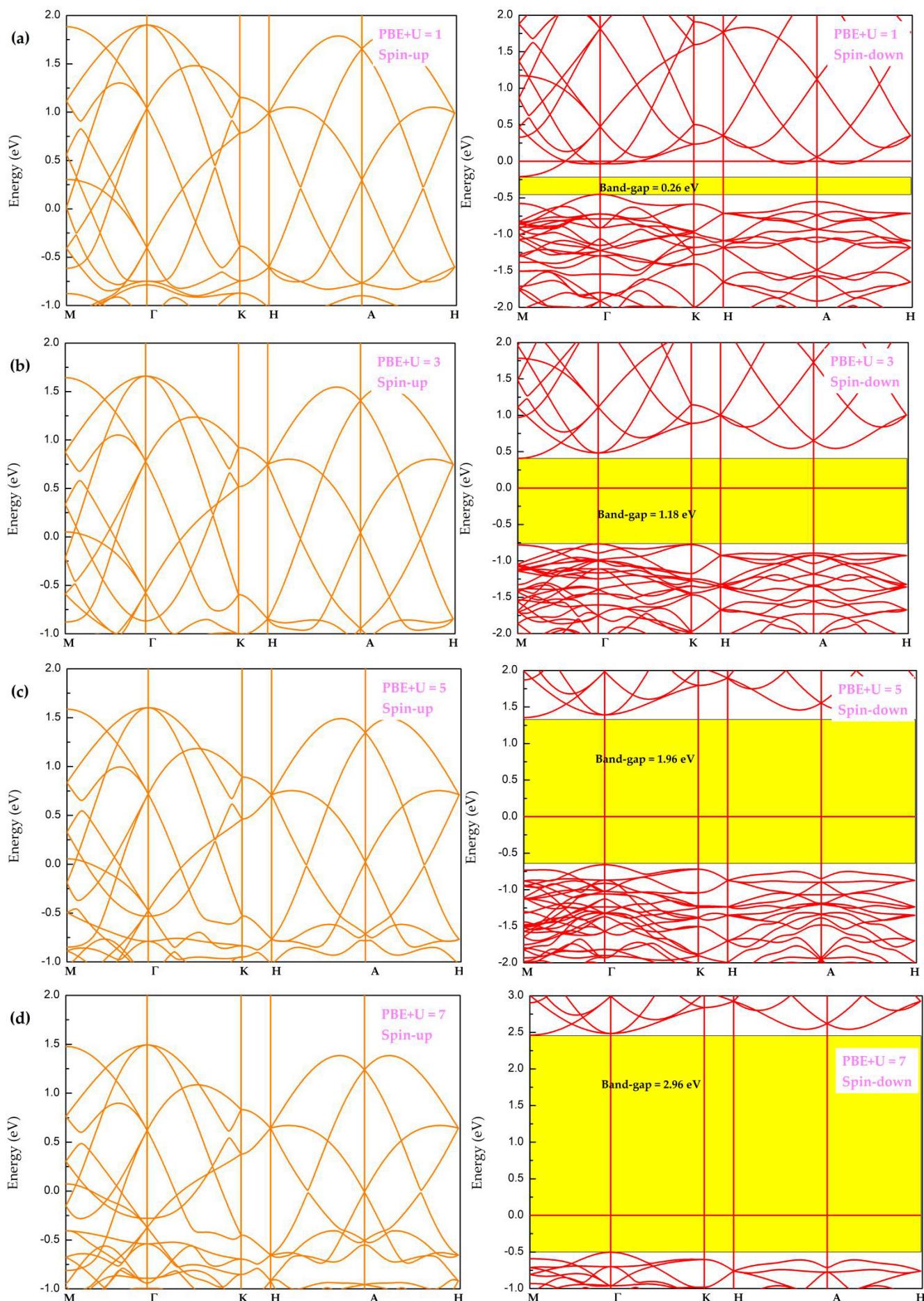


Figure S1. Crystal structures of LaNiO_3 material in space group $R\bar{3}c$.

Figure S2 The calculated band structures of LaNiO_3 material under different U values.

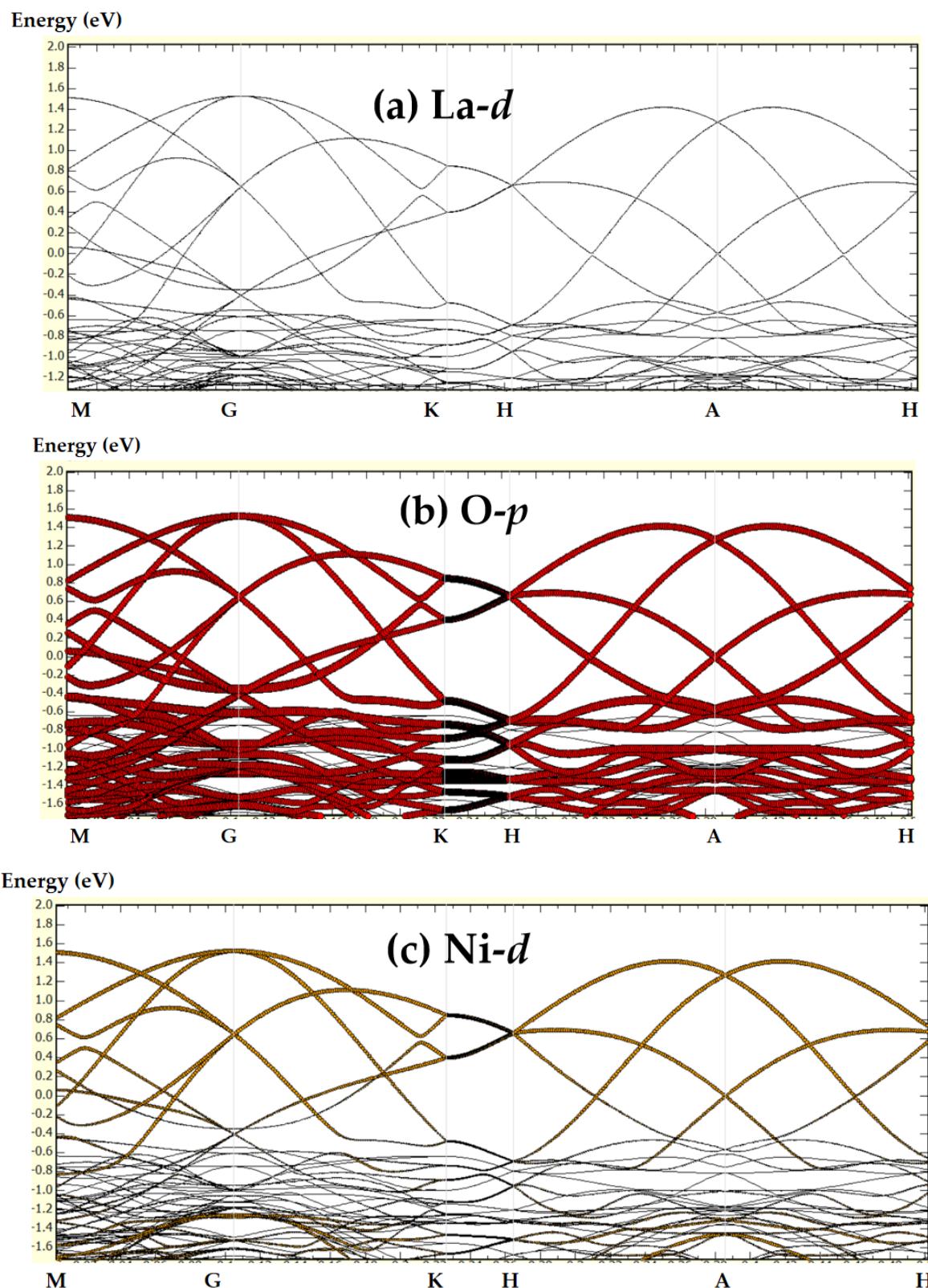
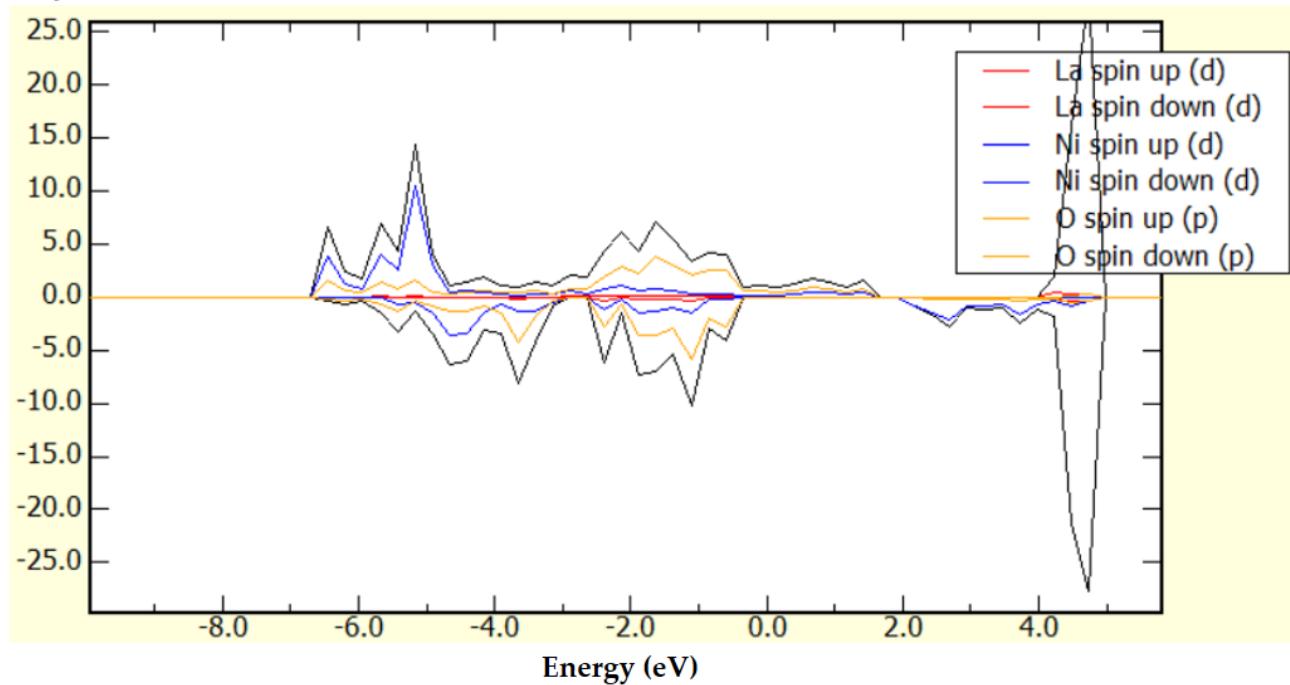


Figure S3 Orbital-resolved band structures for LaNiO_3 contributed by the O-*p*, La-*d*, and Ni-*d* orbits. The thicker line means a higher contribution, while the thinner line indicates a lower contribution.

Density (states/eV)*Figure S4. Calculated total and atomic DOSs for LaNiO_3 .*

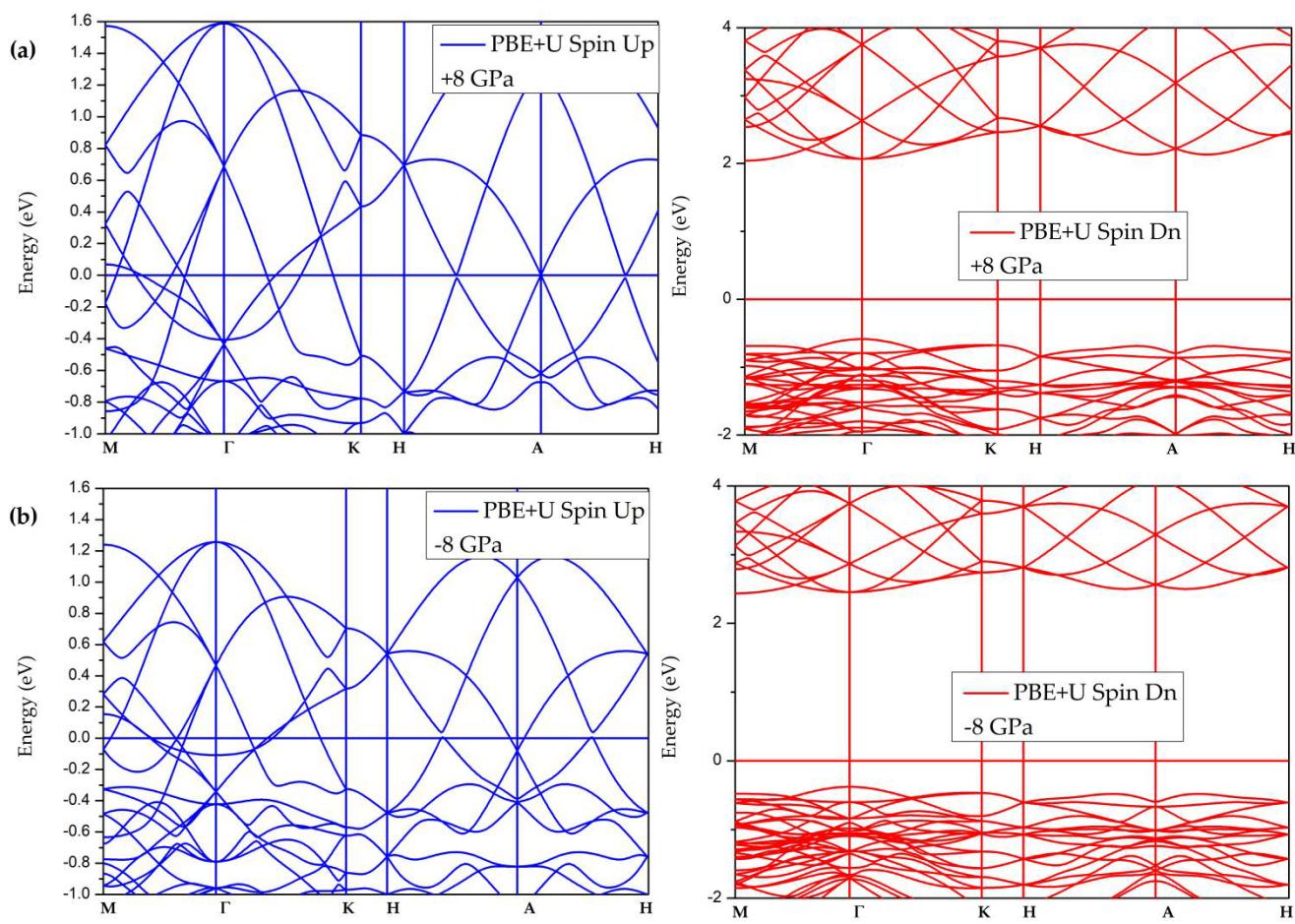


Figure S5. Calculated band structures for LaNiO_3 under +8 GPa and -8 GPa.

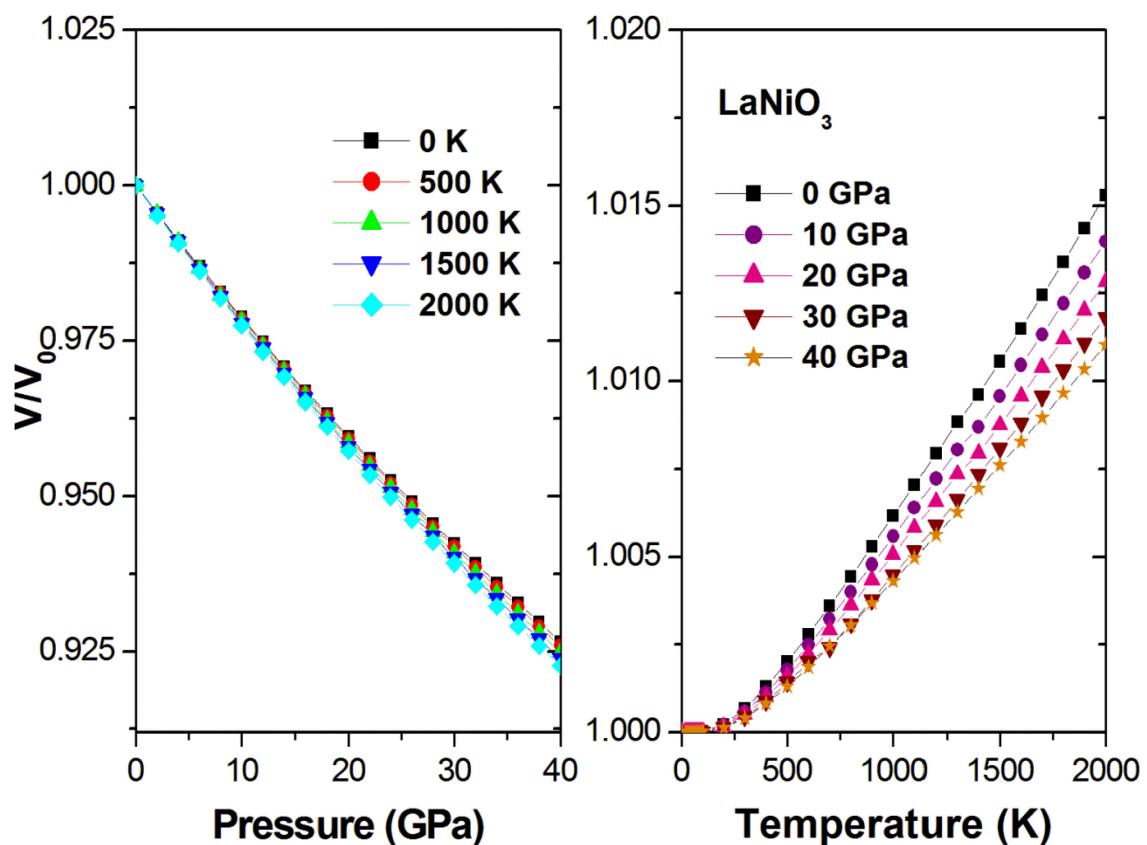


Figure S6 The normalized volume V/V_0 versus pressure and temperature for LaNiO_3 .

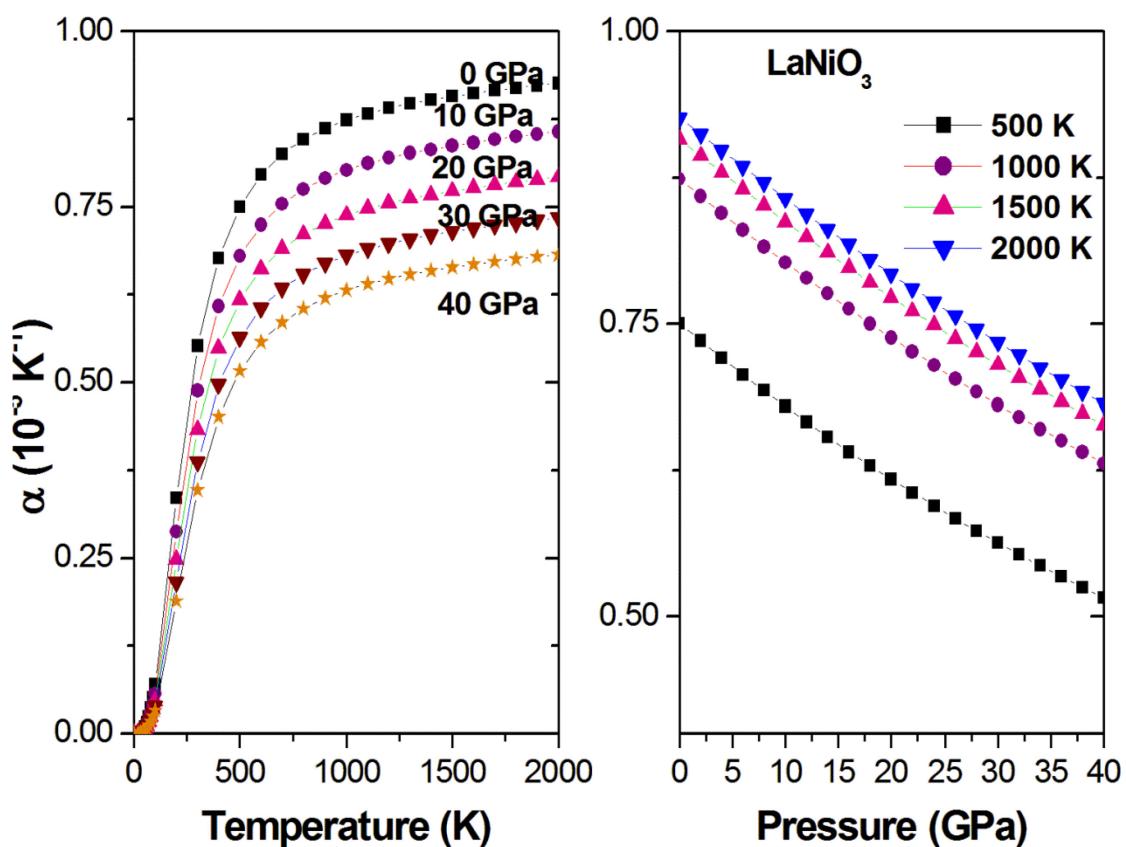


Figure S7. The thermal expansivity α versus pressure and temperature for LaNiO₃.

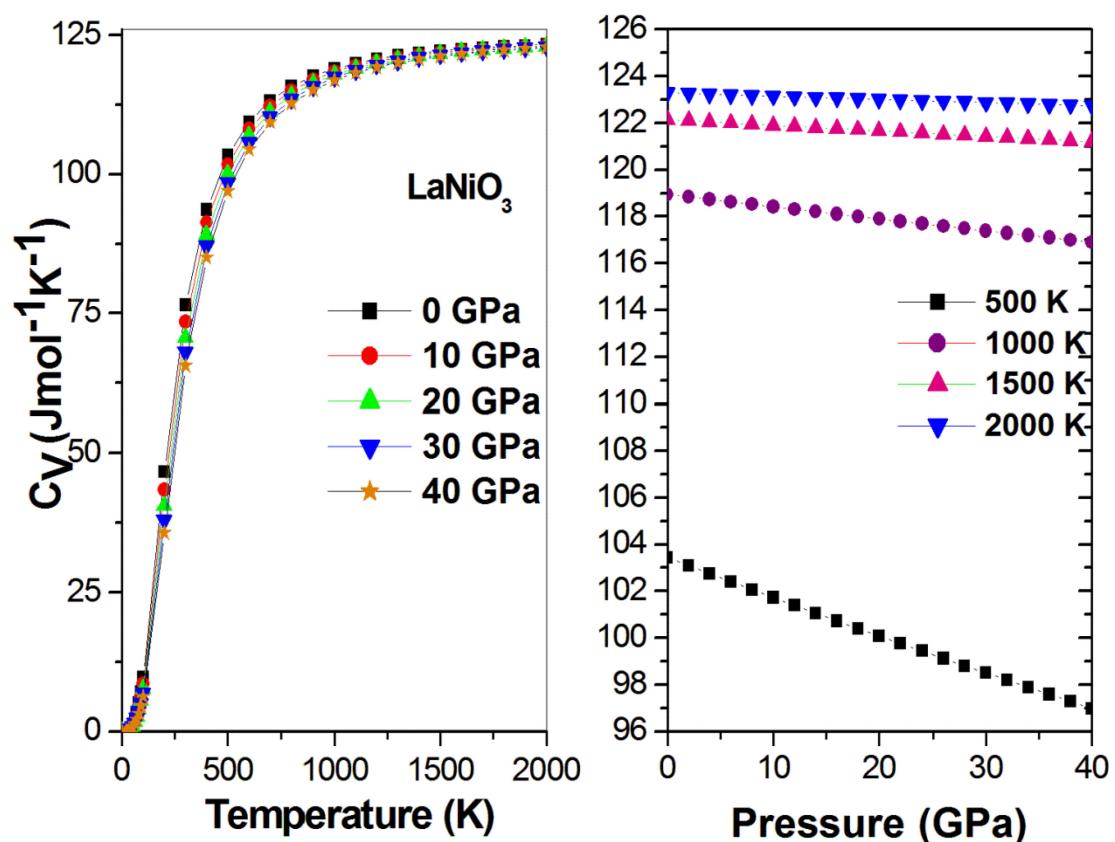


Figure S8 The heat capacity C_V versus temperature and pressure for LaNiO_3 .

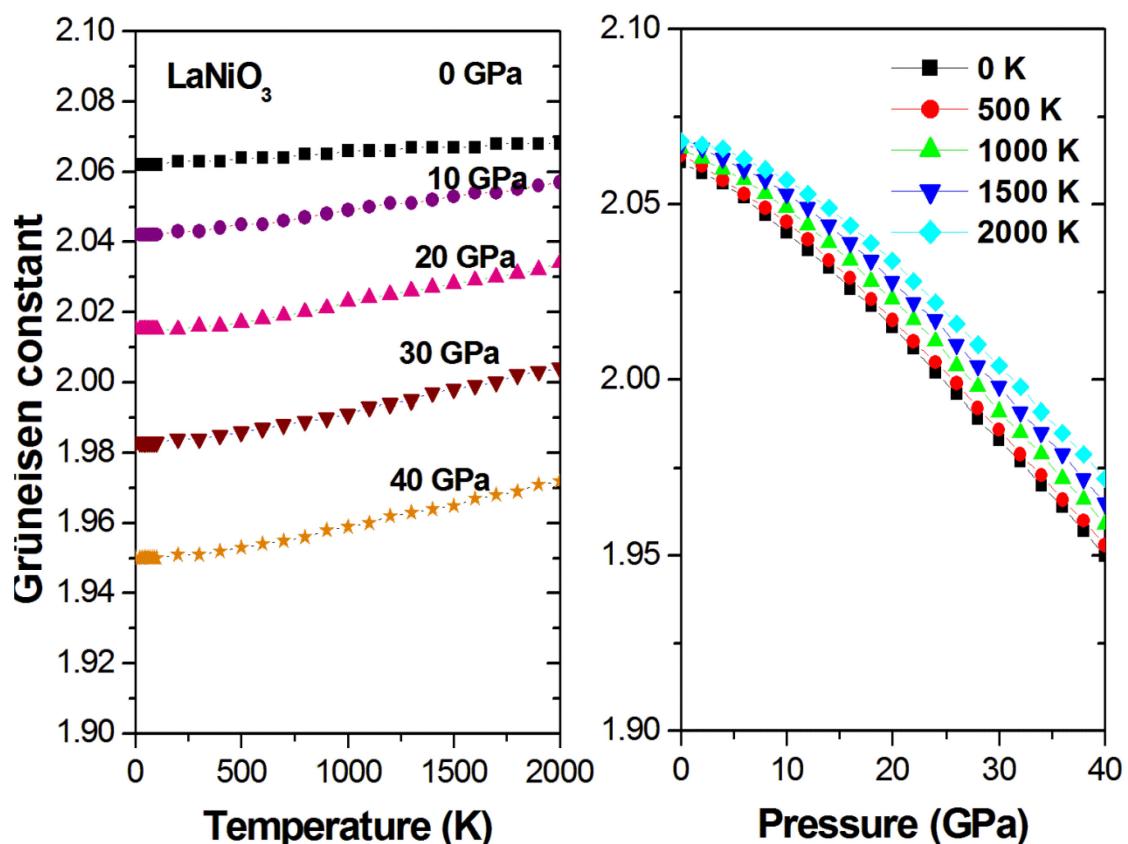


Figure S9 The Grüneisen constant γ versus pressure and temperature for LaNiO_3 .

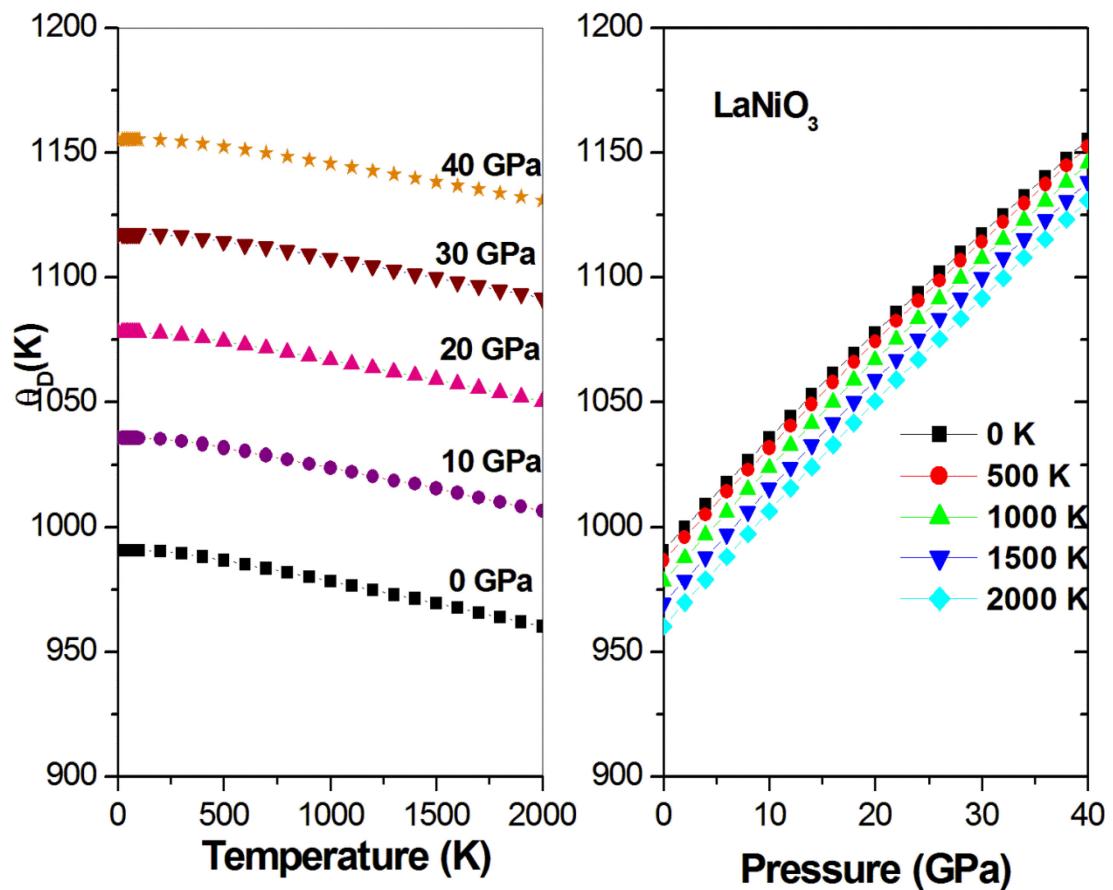


Figure S10 The Debye temperature Θ_D versus pressure and temperature for LaNiO_3 .

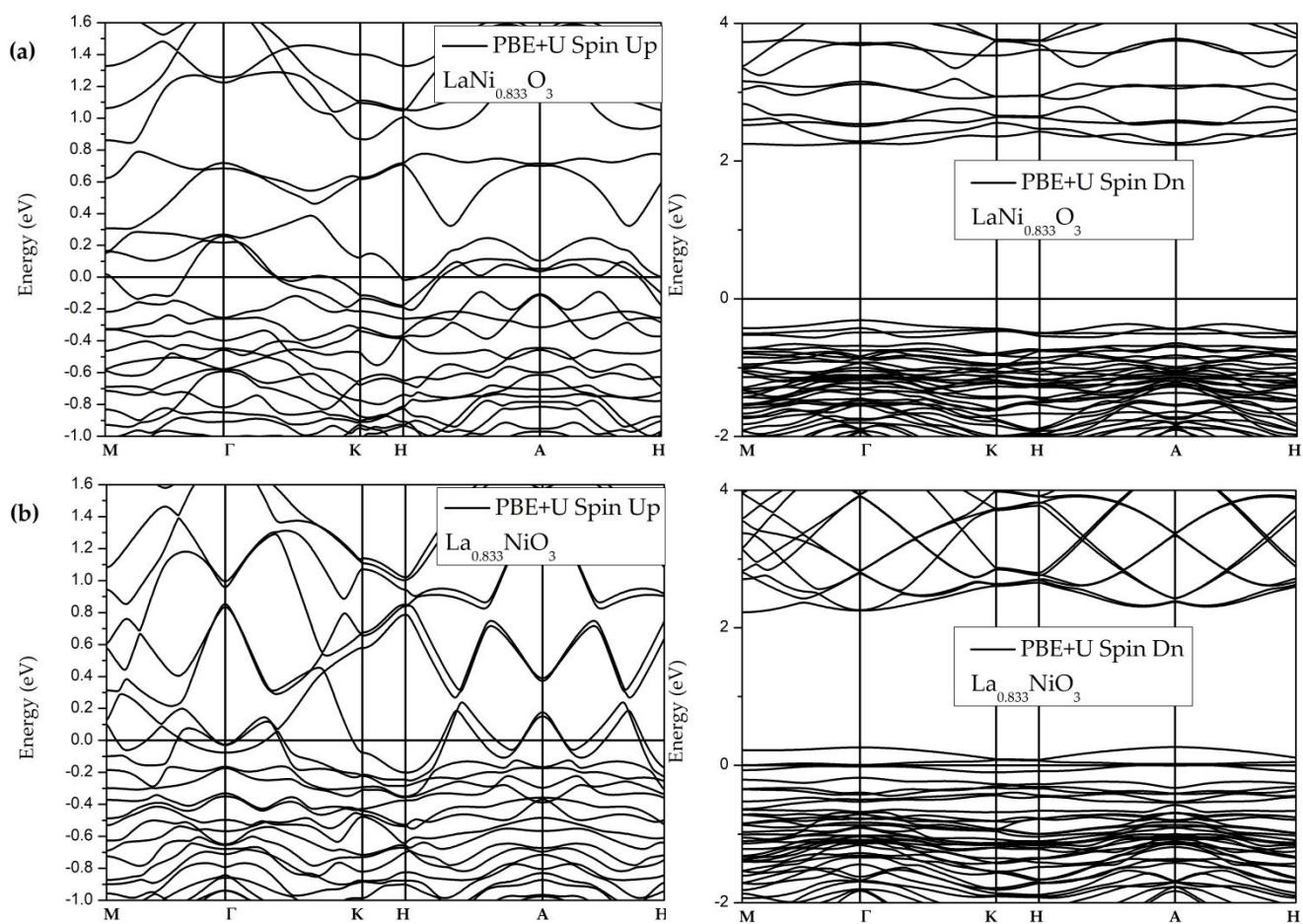


Figure S11. Calculated band structures of $\text{La}_{0.833}\text{NiO}_3$ and $\text{LaNi}_{0.833}\text{O}_3$ in both spin channels.

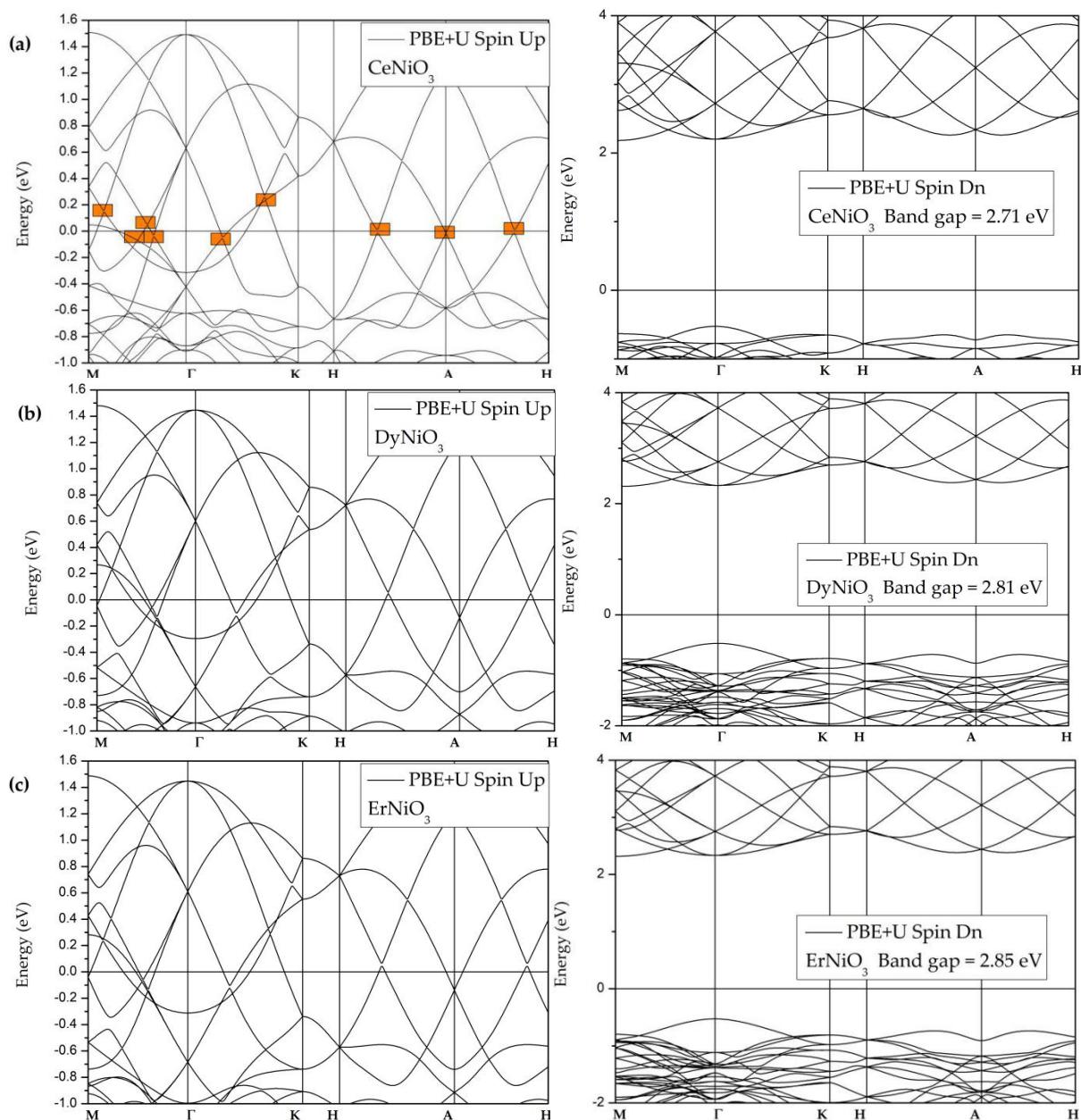


Figure S12. Cont.

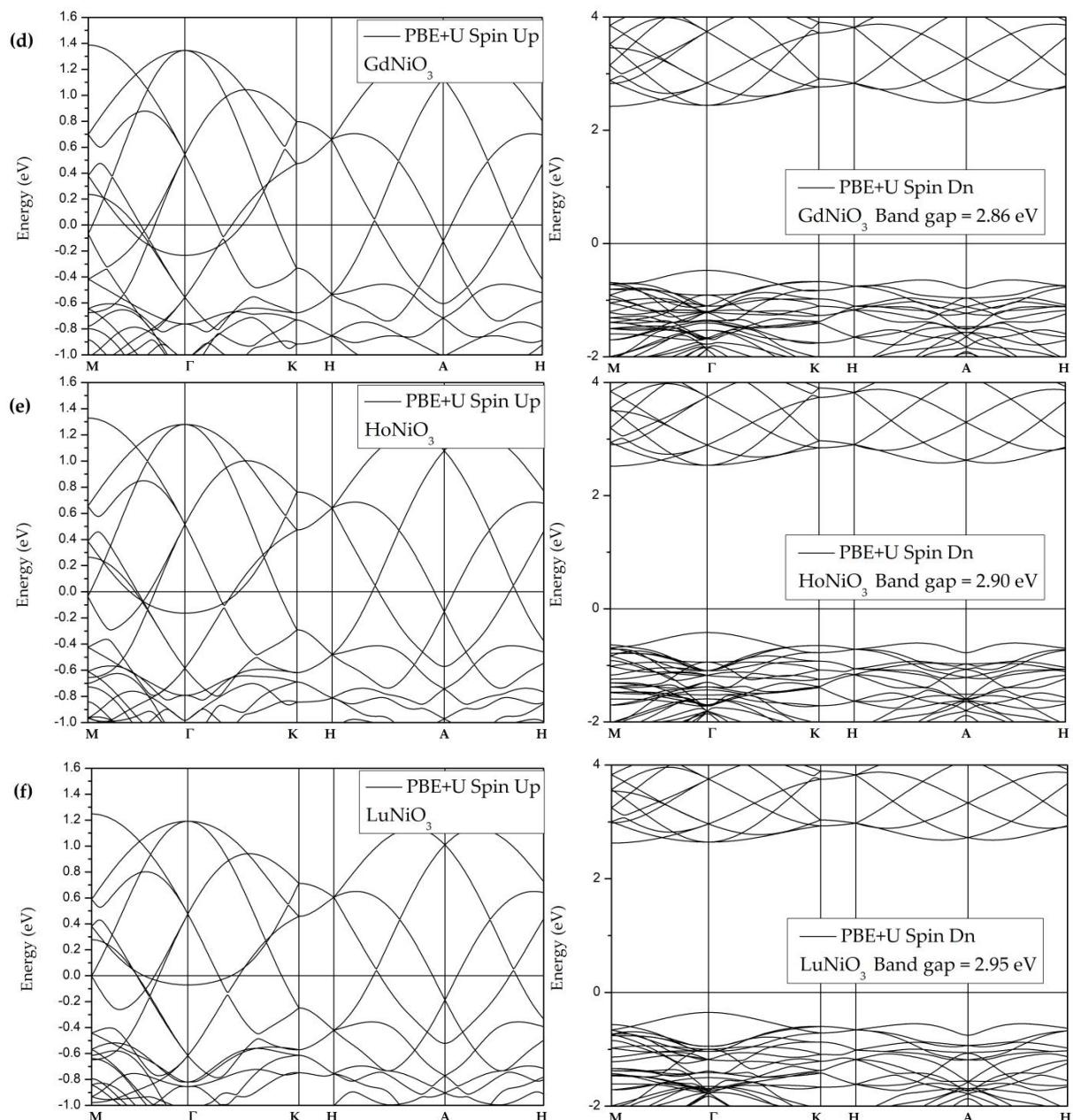


Figure S12. Cont.

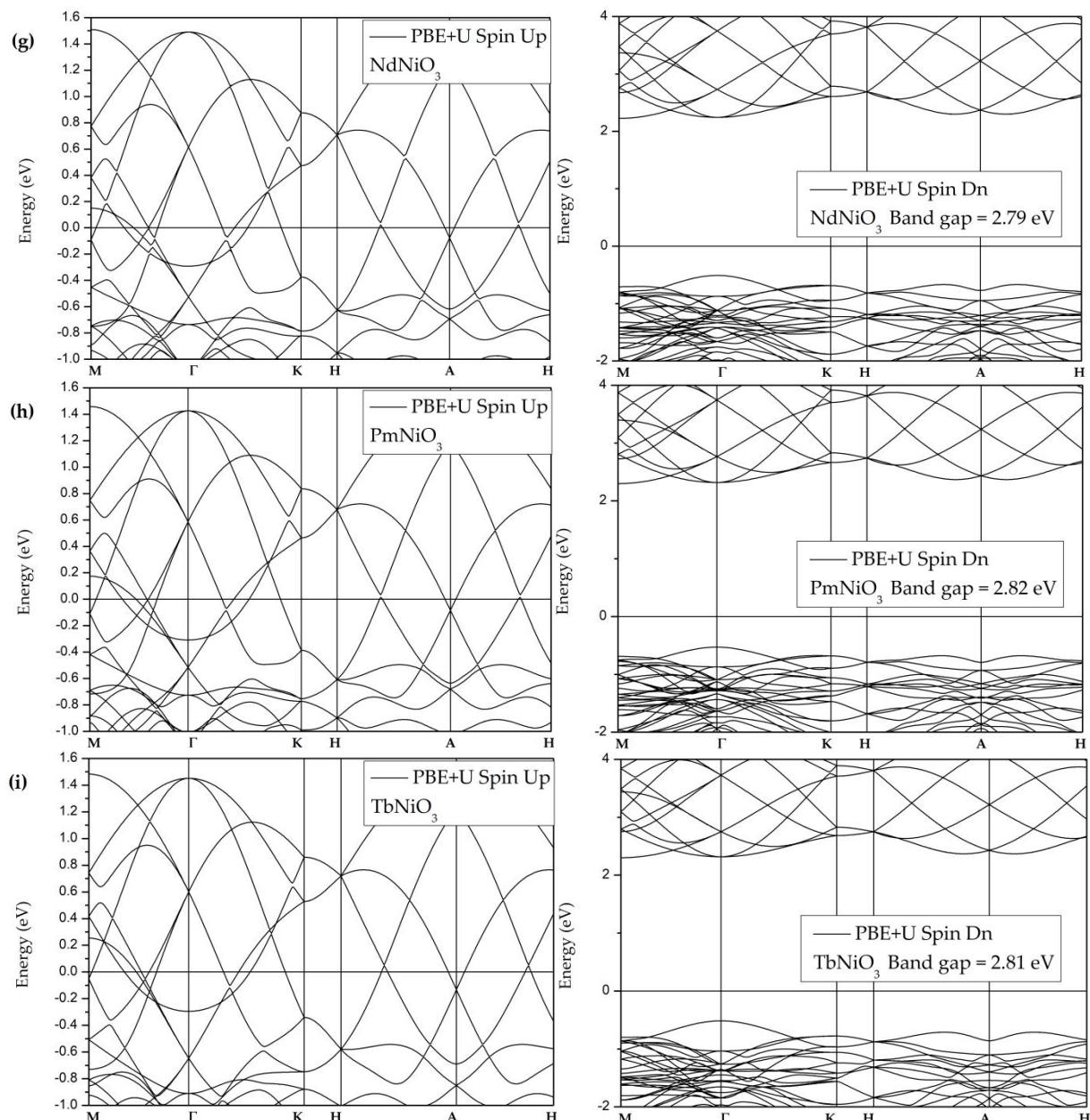


Figure S12. Calculated band structures of a series of $R\bar{3}c$ -based DHMs with MDRs $LnNiO_3$ ($Ln = Ce, Nd, Pm, Gd, Tb, Dy, Ho, Er, Lu$).

Table S1. Characters table for irreducible representations of the D_{3d} point group.

	E	$2C_3$	$3C'_2$	i	$2S_6$	$3\sigma_d$
A_{1g}	1	1	1	1	1	1
A_{2g}	1	1	-1	1	1	-1
E_g	2	-1	0	2	-1	0
A_{1u}	1	1	1	-1	-1	-1
A_{2u}	1	1	-1	-1	-1	1
E_u	2	-1	0	-2	1	0