

Accurate projected augmented wave (PAW) datasets for rare-earth elements (RE=La-Lu): supplementary material

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Table I: Cubic lattice constant (a_0), bulk modulus (B_0) and total magnetic moments (μ_0) of REN's calculated with all-electron (AE) and PAW (see text).

Element	a_{0-AE} (a.u.)	a_{0-PAW} (a.u.)	B_{0-AE} (GPa)	B_{0-PAW} (GPa)	μ_{0-AE} (μ_B)	μ_{0-PAW} (μ_B)
La	10.0457	10.0465	122	122	0.00	0.00
Ce	9.5612	9.5609	145	150	0.27	0.40
Pr	9.5888	9.5898	120	123	1.93	1.91
Nd	9.6424	9.6432	123	122	3.00	3.00
Pm	9.5234	9.5237	137	132	4.00	4.00
Sm	9.5177	9.5191	122	126	5.00	5.00
Eu	9.5435	9.5451	117	119	6.00	6.00
Gd	9.4306	9.4317	143	147	7.00	7.00
Tb	9.2739	9.2746	140	142	6.03	6.05
Dy	9.2383	9.2401	143	145	5.01	5.01
Ho	9.2233	9.2235	151	152	4.00	4.00
Er	9.1641	9.1661	147	149	3.00	3.00
Tm	9.1124	9.1123	143	146	1.93	1.90
Yb	9.0795	9.0810	140	145	0.22	0.14
Lu	9.0103	9.0108	170	171	0.00	0.00

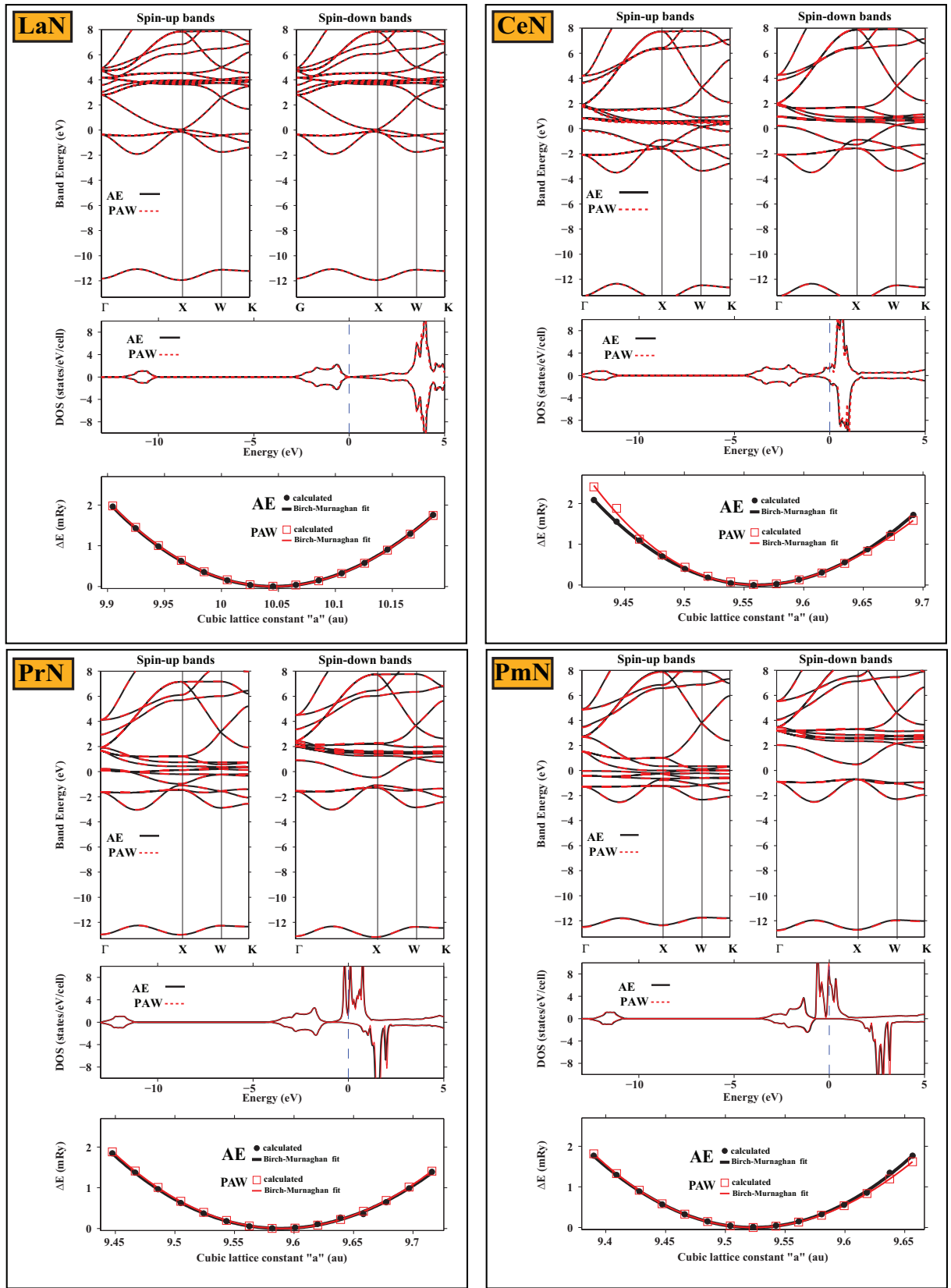


Figure 1: (Color online) Band structure, density of states (DOS) and equation of state (EoS) comparison of PAW with all-electron (AE) calculations for LaN, CeN, PrN, PmN.

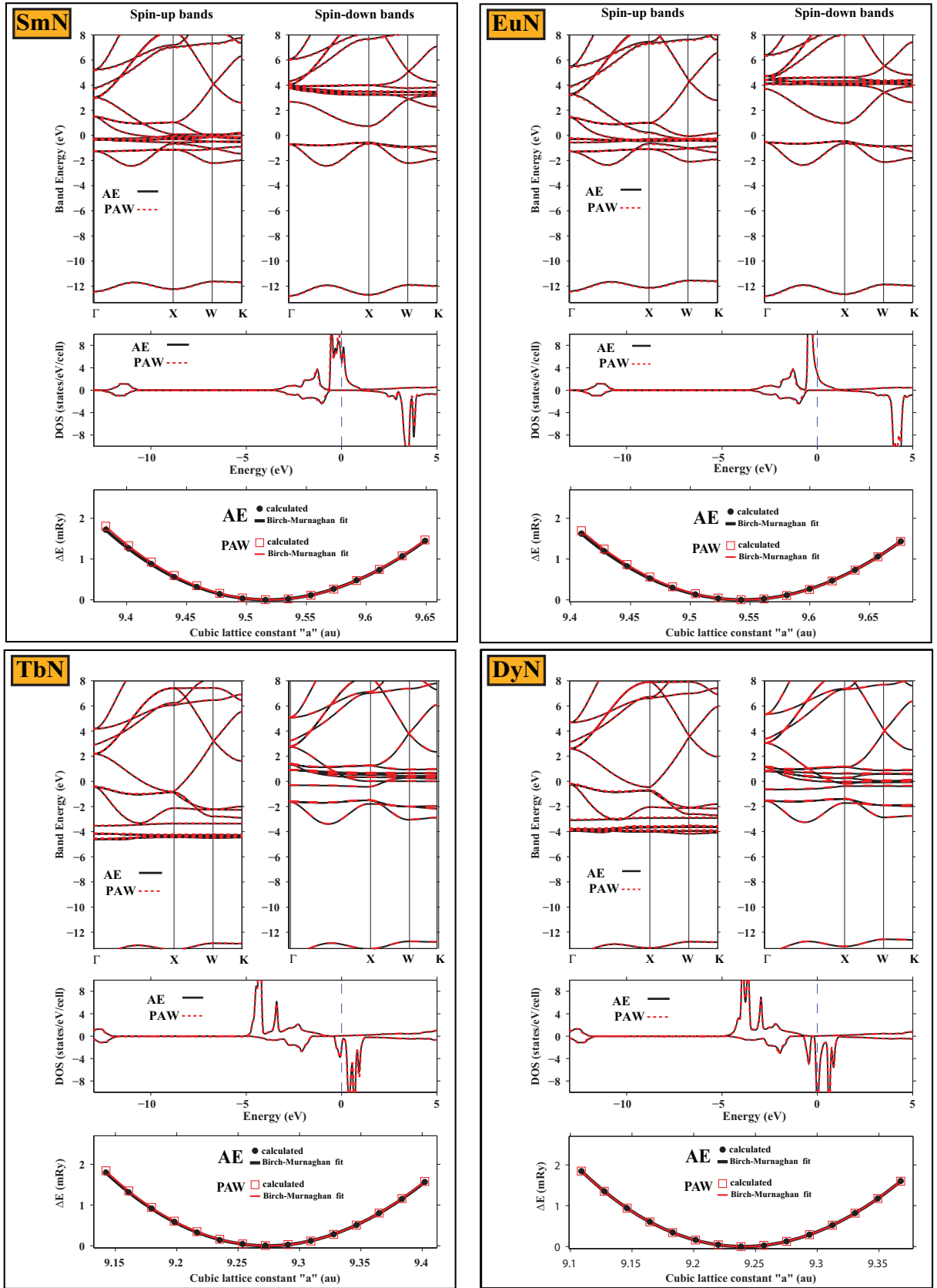


Figure 2: (Color online) Band structure, density of states (DOS) and equation of state (EoS) comparison of PAW with all-electron (AE) calculations for SmN, EuN, TbN, DyN.

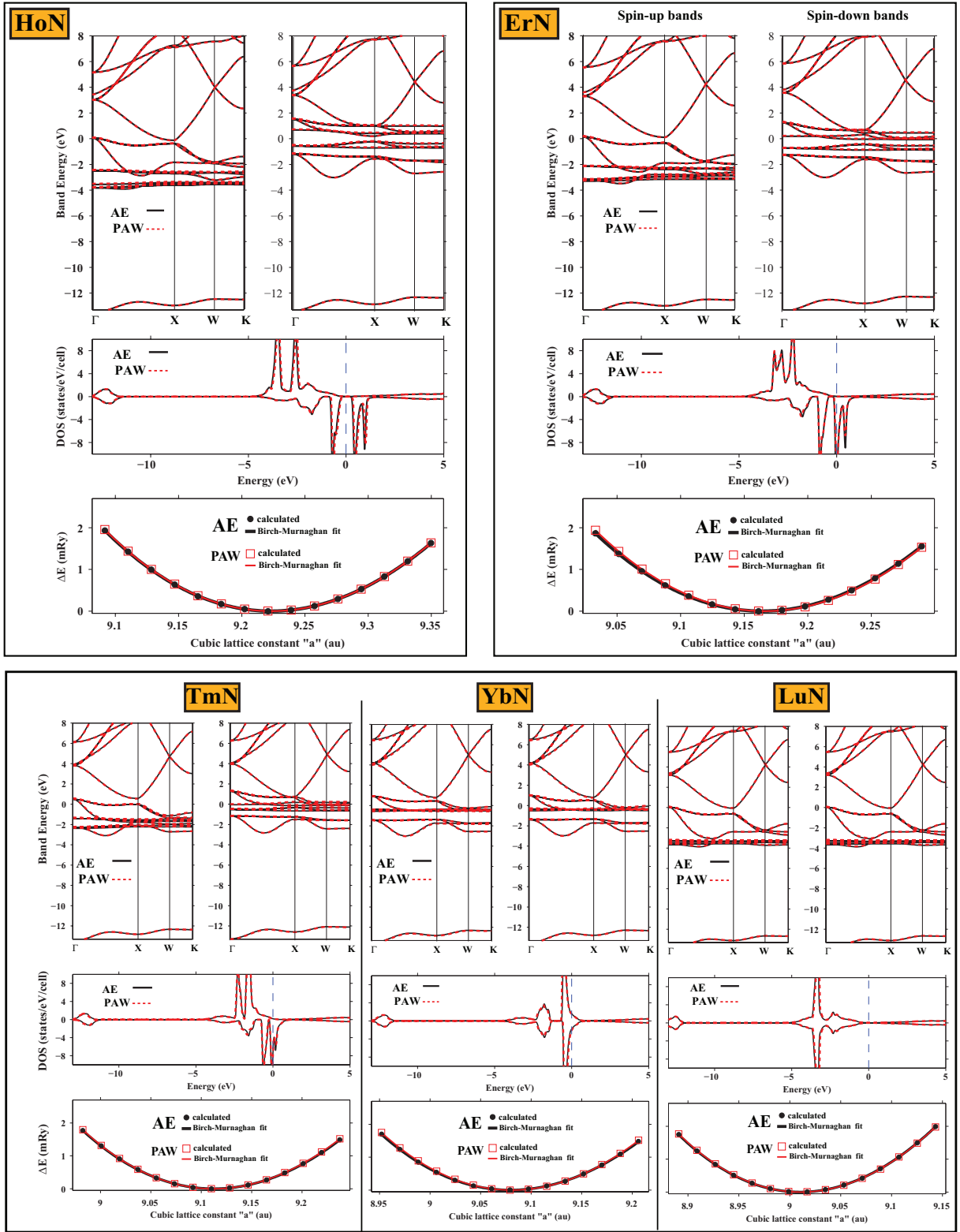


Figure 3: (Color online) Band structure, density of states (DOS) and equation of state (EoS) comparison of PAW with all-electron (AE) calculations for HoN, ErN, TmN, YbN, LuN.