

Supplementary Information for “Prediction of Ambient Pressure Conventional Superconductivity above 80 K in Hydride Compounds”

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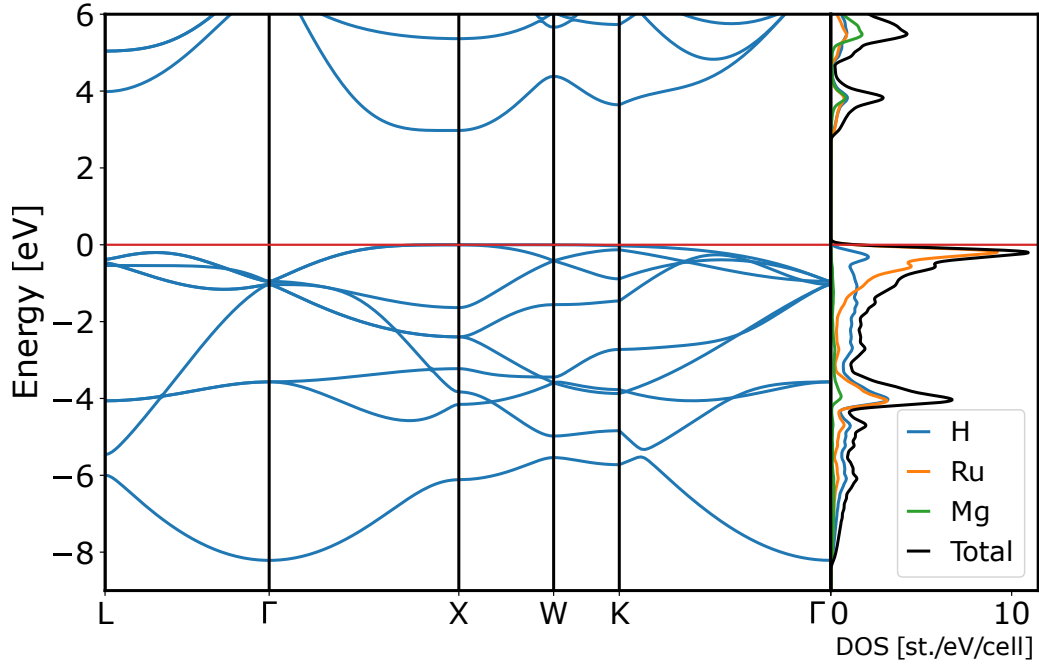
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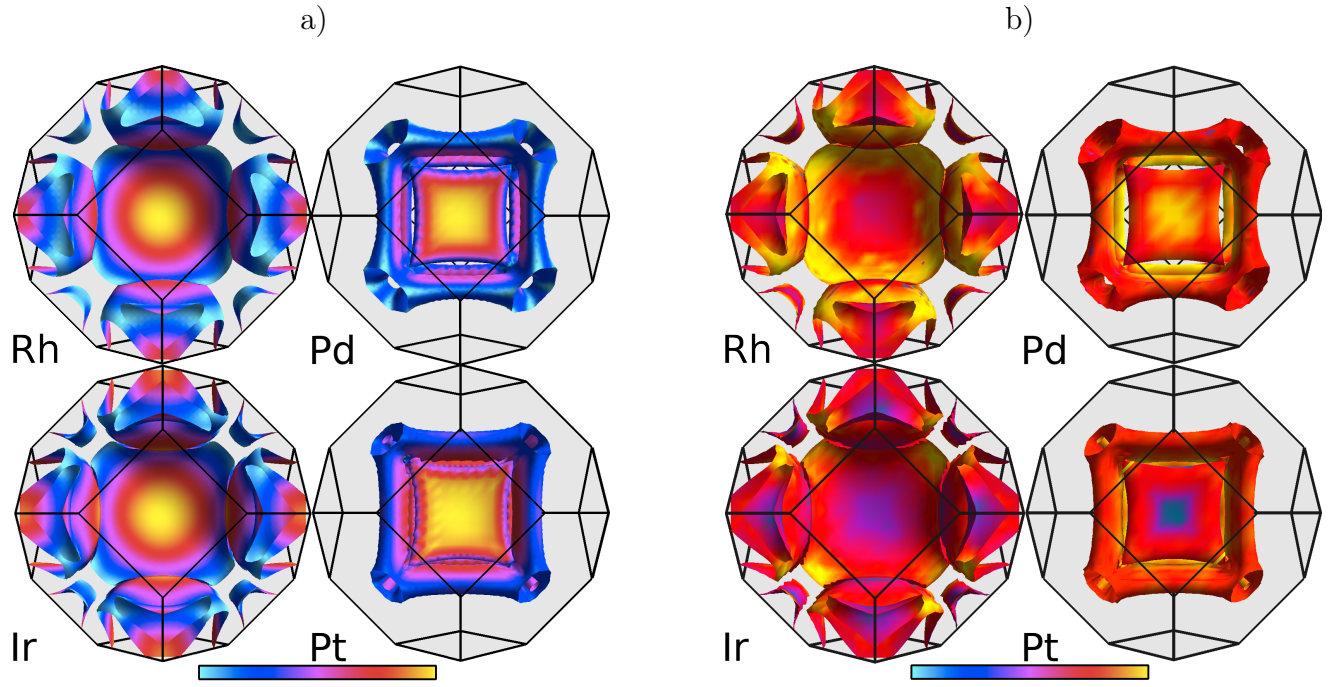
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Supplementary Figure 1. Bandstructure and DOS for the semiconducting Mg_2RuH_6 .

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Supplementary Figure 2. Fermi surfaces of the Mg_2XH_6 compounds studied in this work. On the left, (a), the surface color indicates the Fermi velocity, from light-blue (low) to yellow (high). On the right, (b), the surface color indicates the superconducting gap from light blue (low) to yellow (high). The energy range of the superconducting gap is 7-9.5, 9-11, 10.5-14.5, 12.5-15 meV for the Rh, Pd, Ir and Pt compounds respectively.

PBEsol structures of Mg_2XH_6 in the VASP format

a. Mg_2PtH_6

Mg2 H6 Pt1

1.0

4.0349872673825020	0.0000000000000000	2.3296009850000003
1.3449957557941674	3.8042224783567256	2.3296009850000003
0.0000000000000000	0.0000000000000000	4.6592019699999998

Mg H Pt

2 6 1

direct

0.2500000000000000	0.2500000100000000	0.2500000000000000	Mg
0.7500000000000000	0.7500000100000001	0.7499999899999999	Mg
0.2714615200000000	0.7285384800000000	0.7285384800000000	H
0.2714615200000000	0.7285384800000000	0.2714615300000000	H
0.7285384800000000	0.7285384800000000	0.2714615200000000	H
0.7285384700000000	0.2714615300000000	0.2714615300000000	H
0.7285384700000000	0.2714615300000000	0.7285384700000000	H
0.2714615300000000	0.2714615300000000	0.7285384700000000	H
0.0000000000000000	0.0000000000000000	0.0000000000000000	Pt

b. Mg_2PdH_6

Mg2 H6 Pd1

1.0

4.0145472665203492	0.0000000000000000	2.3177999450000004
1.3381824221734500	3.7849514607339425	2.3177999450000004
0.0000000000000000	0.0000000000000000	4.6355998899999999

Mg H Pd

2 6 1

direct

0.2500000000000000	0.2500000100000000	0.2500000000000000	Mg
0.7500000000000000	0.7500000100000001	0.7499999899999999	Mg
0.2712766800000000	0.7287233200000000	0.7287233200000000	H
0.2712766800000000	0.7287233200000000	0.2712766800000000	H
0.7287233200000000	0.7287233200000000	0.2712766800000000	H
0.7287233200000000	0.2712766800000000	0.2712766800000000	H
0.7287233100000000	0.2712766900000000	0.7287233200000000	H
0.2712766800000000	0.2712766900000000	0.7287233200000000	H
0.0000000000000000	0.0000000000000000	0.0000000000000000	Pd

c. Mg_2IrH_6

Mg2 H6 Ir1

1.0

4.0375223922072543	0.0000000000000000	2.3310646400000006
1.3458407974024182	3.8066126169630410	2.3310646400000006
0.0000000000000000	0.0000000000000000	4.6621292800000003

Mg H Ir

2 6 1

direct

0.2500000000000000	0.2500000100000000	0.2500000000000000	Mg
0.7500000000000000	0.7500000100000001	0.7499999899999999	Mg
0.2603496100000000	0.7396503900000000	0.7396503900000000	H
0.2603496100000000	0.7396503900000000	0.2603496200000000	H
0.7396503900000000	0.7396503900000000	0.2603496100000000	H
0.7396503800000001	0.2603496200000000	0.2603496200000000	H
0.7396503800000001	0.2603496200000000	0.7396503800000001	H
0.2603496200000000	0.2603496200000000	0.7396503800000001	H
0.0000000000000000	0.0000000000000000	0.0000000000000000	Ir

d. Mg₂RhH₆

Mg2 H6 Rh1

1.0

4.0111743400597222	0.0000000000000000	2.3158525850000005
1.3370581133532409	3.7817714351702723	2.3158525850000005
0.0000000000000000	0.0000000000000000	4.6317051700000000

Mg H Rh

2 6 1

direct

0.2500000000000000	0.2500000100000000	0.2500000000000000 Mg
0.7500000000000000	0.7500000100000001	0.7499999899999999 Mg
0.2600665600000000	0.7399334400000001	0.7399334400000001 H
0.2600665600000000	0.7399334400000001	0.2600665700000000 H
0.7399334400000001	0.7399334400000001	0.2600665600000000 H
0.7399334300000000	0.2600665700000000	0.2600665700000000 H
0.7399334300000000	0.2600665700000000	0.7399334300000000 H
0.2600665700000000	0.2600665700000000	0.7399334300000000 H
0.0000000000000000	0.0000000000000000	0.0000000000000000 Rh