Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information for "Prediction of Pressure-induced Phase Transformations in Mg_3As_2"

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We calculated electronic band structures (PBE) of Mg_3As_2 compound for (a) the $Ia\bar{3}$ phase at ambient pressure, (b) the $P\bar{3}m1$ phase at 1.5 GPa, (c) the $C2/m$ phase at 20 GPa and (d) the $P\bar{1}$ phase at 30 GPa, respectively. As shown in Figure S1. Three-dimensional electron localization function of all structures are shown in Figure S2. Charge density difference plots of all structures are shown in Figure S3.

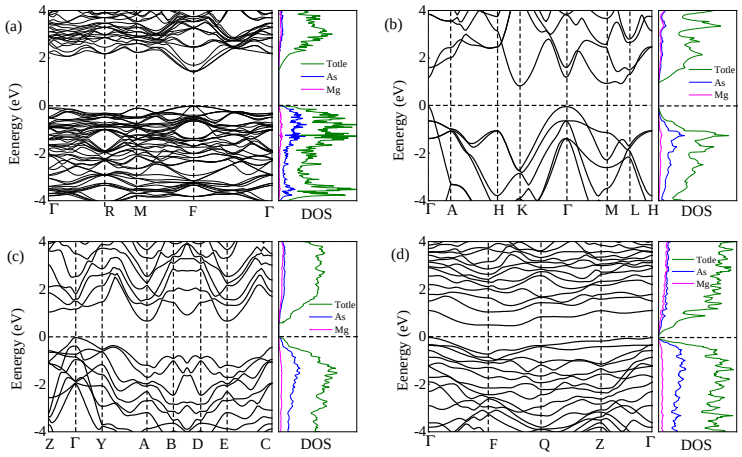

Figure S1: (a) Calculated electronic band structures (PBE) of Mg_3As_2 for (a) the $Ia\bar{3}$ phase at ambient pressure, (b) the $P\bar{3}m1$ phase at 1.5 GPa, (c) the $C2/m$ phase at 20 GPa and (d) the $P\bar{1}$ phase at 30 GPa.

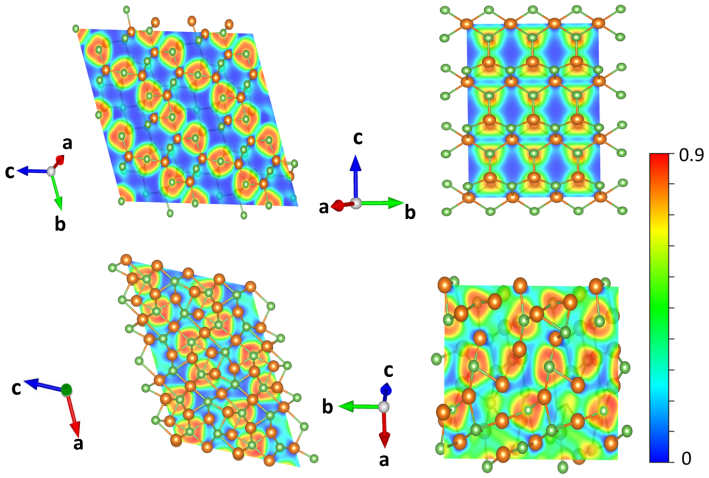

Figure S2: Three-dimensional electron localization function with isosurface value of 0.9 of (a) the $Ia\bar{3}$ phase at ambient pressure, (b) the $P\bar{3}m1$ phase at 1.5 GPa, (c) the $C2/m$ phase at 20 GPa and (d) the $P\bar{1}$ phase at 30 GPa, respectively.

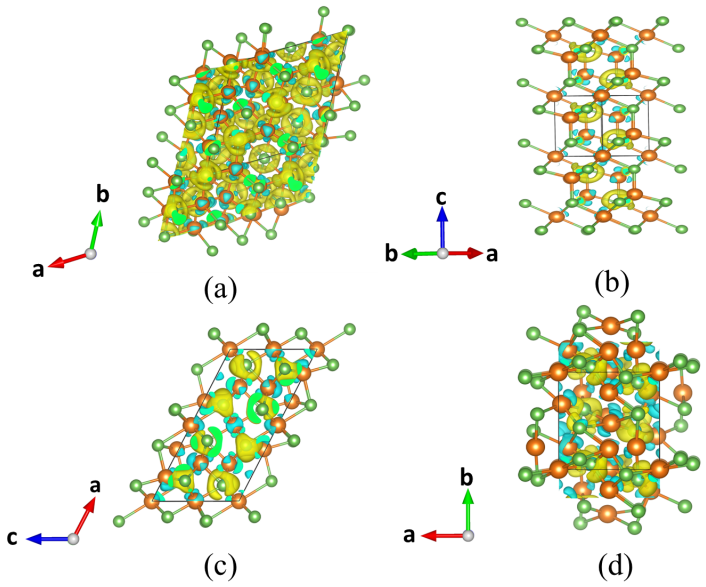

Figure S3: Charge density difference plot of (a) the $Ia\bar{3}$ phase at ambient pressure, (b) the $P\bar{3}m1$ phase at 1.5 GPa, (c) the $C2/m$ phase at 20 GPa and (d) the $P\bar{1}$ phase at 30 GPa, respectively.