SUPPLEMENTARY MATERIAL

Volume Expansive Pressure (VEP) Driven Non-Trivial Topological Phase Transition In LiMgBi

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Computational Details:

To get accurate band gap we have done simulations using the density functional theory based projector augmented wave (PAW) method as implemented in the VASP code [1, 2, 3, 4]. The cut-off for the plane-wave basis expansion is taken as 500eV. To sample the brillioun zone we have used a Monkhorst pack [5] mesh of $6 \times 6 \times 6$ **k**-points. We have employed both GGA exchange correlation functional [6] and state-of-the-art hybrid functional based on the Heyd-Scuseria-Ernzerhof (HSE06) functional [7], which gives better description of electronic and magnetic properties. The convergence criterion of 0.01 eV/Å for Hellmann-Feynman forces and 10^6 eV for total energy were considered.

Results

Figure 1 presents the Density of States for 4% VEP using hybrid functional. It is interesting to note that DOS at 4% VEP exhibits a semi-metal character with Dirac cone type signature having zero band gap, justifying our GGA predictions. With increasing VEP to 6.5%, we observe an opening of band gap, consistent to our GGA results. The band gap pattern is almost same for both GGA and hybrid functional calculations.

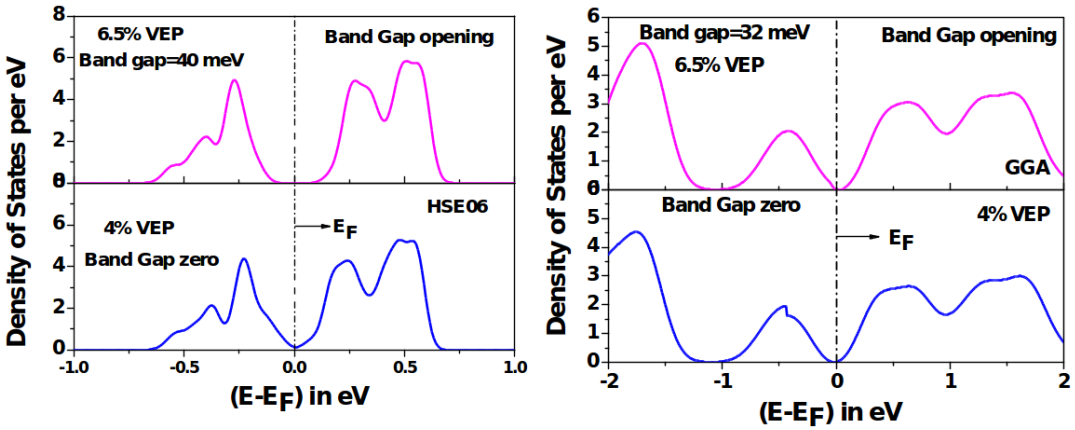

Figure 1: Density of States (DOS) under HSE06 (left) and GGA (right) at 4% VEP(lower panel) and 6.5% VEP; Fermi level is shown by black dotted line.

References

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