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Diverse topological states in ternary compound NdAsPd

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SUPPLEMENTARY MATERIALS

Since that the GGA method often underrates the band gap, we further check the electronic band structure with DFT+U method and nonlocal HSE06 potential, which can better describe the strong correlation effect in the d electrons of transition metal elements. The results are shown in Figure S1 and almost the same band shape, especially for the topological features around the Fermi level, see the insets of the figure, verifying the results of GGA method.

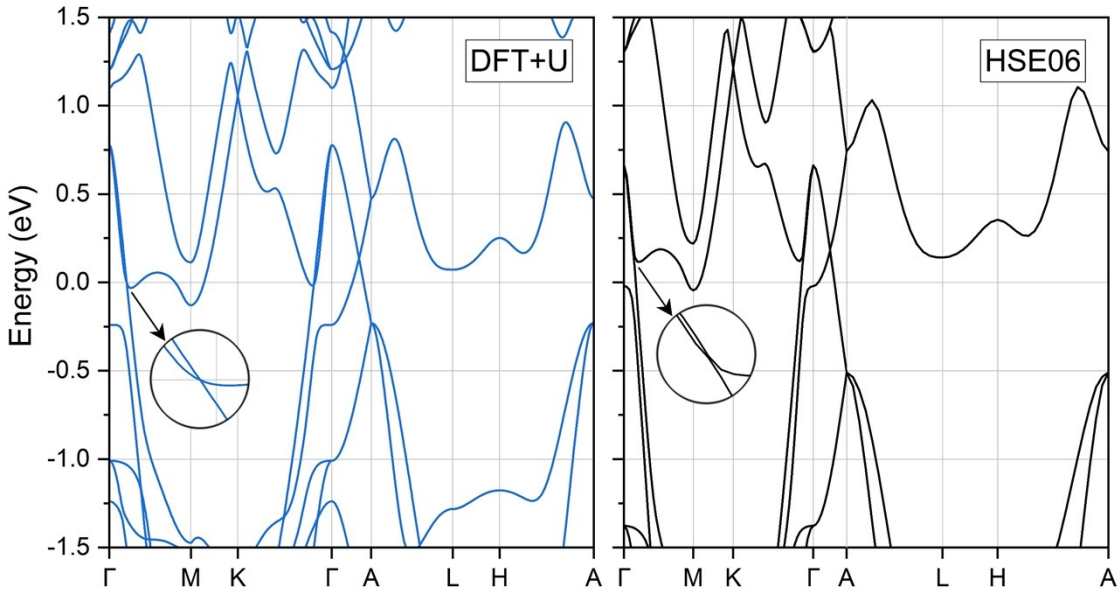

Figure S1 The calculated band structure for NdAsPd with DFT+U method and HSE06 functional.

Table S1: The calculated various elastic constants (C_{ij}), bulk modulus B, Young's modulus E, shear modulus G and Poisson's ratio ν for NdAsPd. All units are in GPa.

C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	B	E	G
246.22	117.18	38.39	90.24	35.56	92.16	125.89	49.47

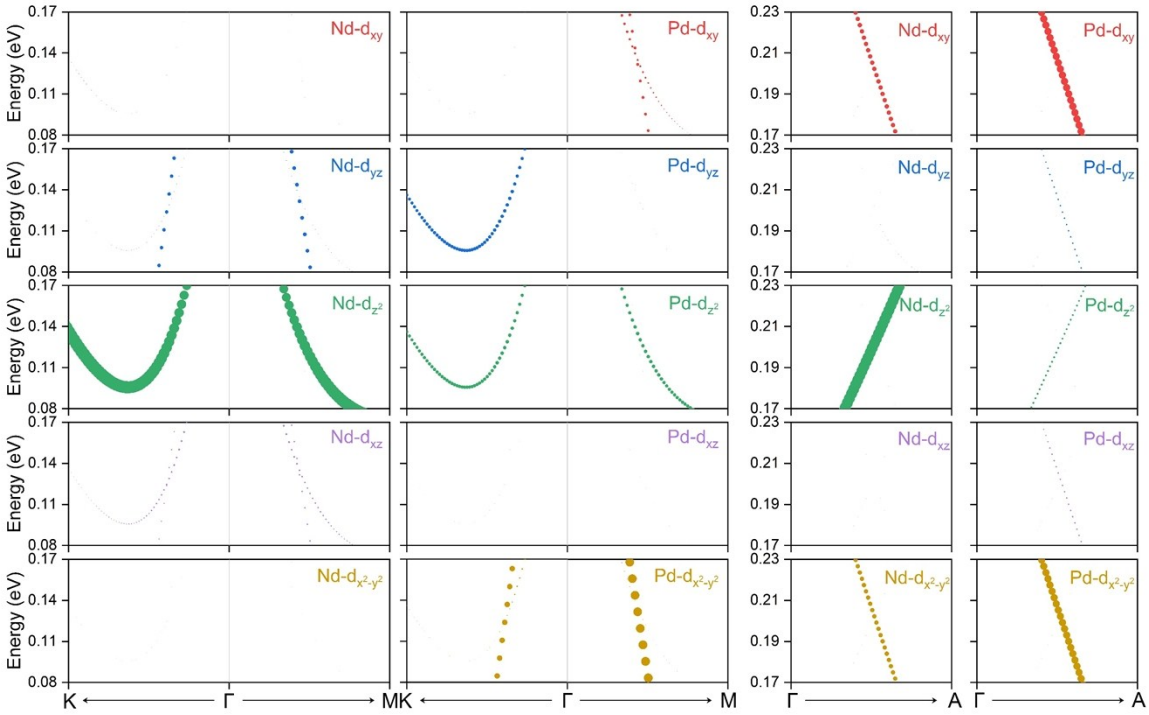

Figure S2 The band crossing areas of NdAsPd with orbital projection for Pd and Nd atoms.

The two crossing bands are mainly contributed from Nd and Pd, a detailed orbital component decomposition is plotted in Figure S2. Only the different orbital projections of *d* electrons have been displayed because the others can be neglected.