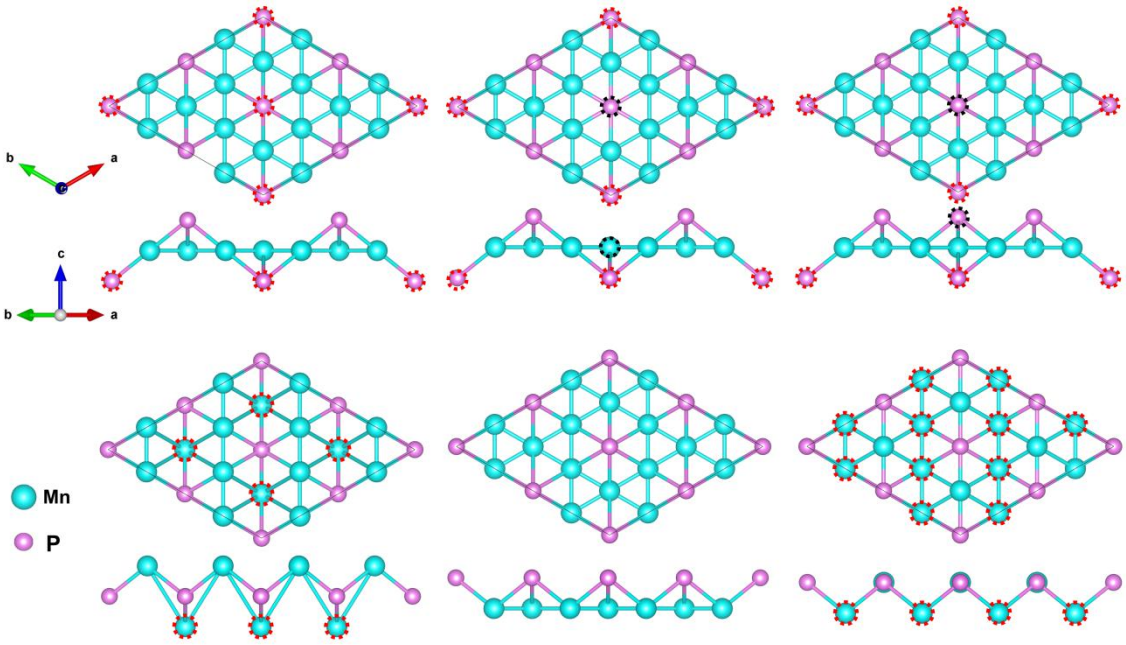
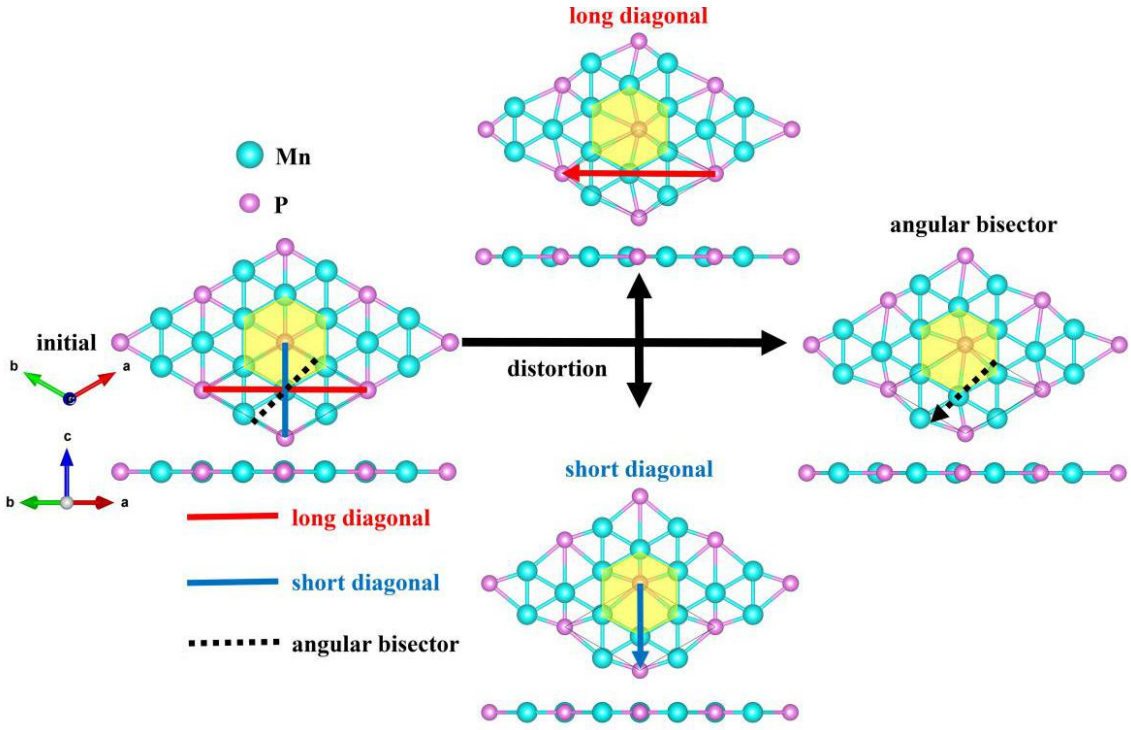
Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Electronic Supplementary Information

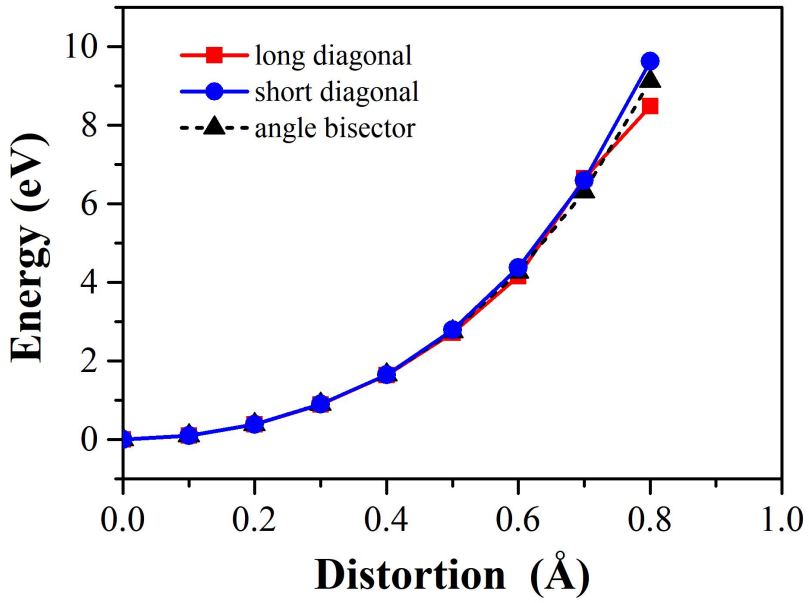


ESI Figure 1 Geometrical structures of bulked 2D Mn_3P monolayer with out-of-plane distortions.



ESI Figure 2 Geometrical structures of 2D Mn_3P monolayer with in-plane distortions, where Mn atoms are shifted with an interval of 0.1 Å along long diagonal, short diagonal, and angular bisector paths indicated in red, blue, and

dashed black arrows, respectively.



ESI Figure 3 Energies of Mn_3P monolayer related to in-plane distortions along long diagonal, short diagonal, and angle bisector paths, respectively.

ESI Table 1 Summary of energy differences for different magnetic configurations of distorted Mn_3P structure obtained from AIMD simulations.

Material	Lattice (Å)	Bond (Å)	Magnetic configuration			ΔE (meV/cell)
Mn_3P	4.60	2.30	FM	Parallel	I) (100)	416.38
					II) (010)	416.42
					III) (001)	437.62
					IV) (110)	416.49
					V) (111)	416.25
			AFM	Antiparallel	VI) rows	232.09
				Chirality	VII) Positive	0
					VIII) Negative	8.95
					IX) Positive and Negative	6.50