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Prediction on the Light-Assisted Exfoliation of Multilayered Arsenene by the Photo-Isomerization of Azobenzene

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Table S1 Force field parameters for C-N=N-C torsion path in the reactive force fields.

system		**torsion path**		
		K_ϕ/kcal·mol^{-1}	n	ϕ_0/°
Default PCFF		7.5	2	180
RMD	*cis to trans*	28	1	0
	trans to *cis*	28	1	180

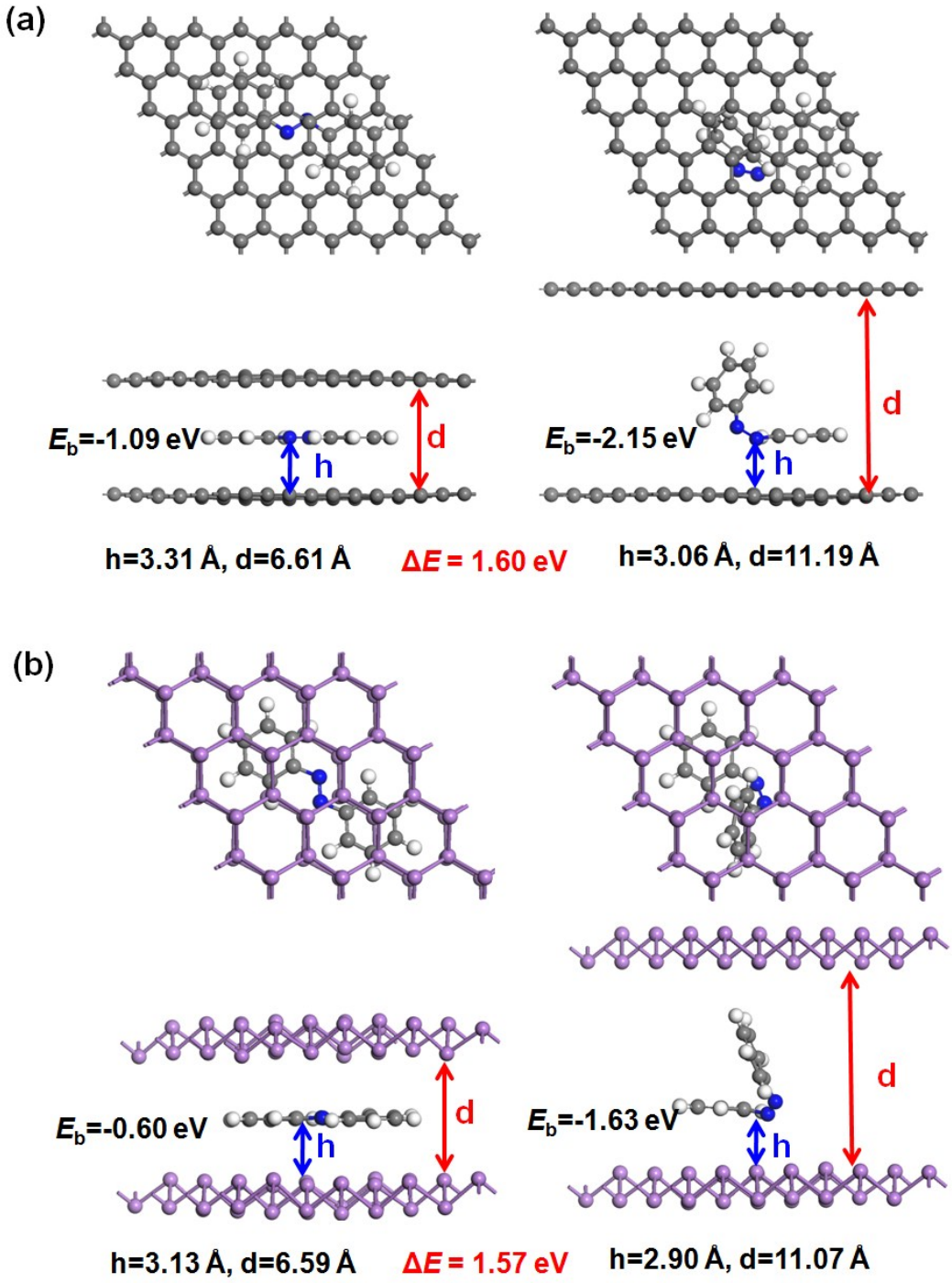

Fig. S1 The optimized structures of *trans*/*cis*-AB sandwiched between (a) two graphene monolayers and (b) two arsenene monolayers. E_b denotes the binding energies of the various hybrid systems.

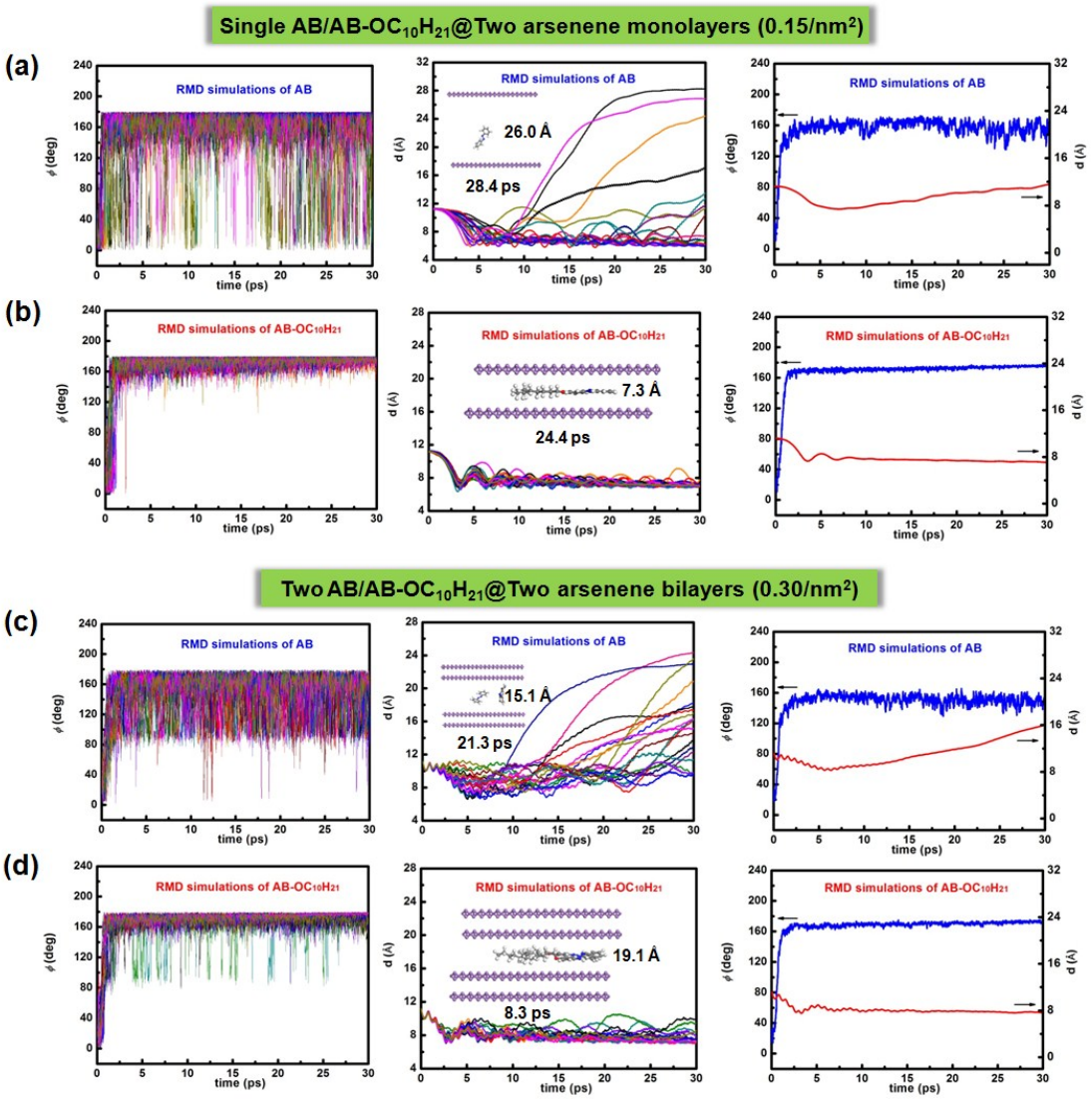

Fig. S2 RMD simulation results of AB-based systems with different layers and coverage rates. The time evolutions of the dihedral angle, ϕ, the interlayer distance, d, and the average dihedral angle along with interlayer distance distributions in twenty independent simulations for (a) single AB and (b) single AB-$OC_{10}H_{21}$ between two arsenene monolayers; (c) two AB and (d) two AB-$OC_{10}H_{21}$ between two arsenene bilayers. Insets in the figure denote the snapshots at different time steps.