

First principles design of two dimensional TiSSe Janus drug delivery system for Nitrosourea

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Table S1. Convergence tests for different energies, k-points, and cut-off energies

system energy (eV)	cutoff energy 300 eV	cutoff energy 500 eV	cutoff energy 550 eV	cutoff energy 600 eV
k-mesh 1×1×1	-345.145	-345.023	-344.985	-345.010
k-mesh 3×3×1	-346.096	-346.027	-346.044	-346.073
k-mesh 5×5×1	-346.197	-346.141	-346.145	-346.174

Table S2. The contribution of vdW interaction energy to stress in the z-axis direction.

configuration	vdW on Z direction (eV)
a	-0.782
b	-1.297
c	-2.291
d	-0.851
e	-1.276
f	-2.232