

## Descriptions of Additional Supplementary Files

File Name: Supplementary Dataset 1

Description: Supplementary Dataset 1 contains geometries in Cartesian coordinates in Å of [123]tetramantane and its dimers computed at the B3LYP-D3(BJ)/6-31G(d,p) level of theory.

File Name: Supplementary Dataset 2

Description: Supplementary Dataset 2 contains geometries in Cartesian coordinates in Å of [123]tetramantane and its dimers computed at the M06-2X/6-31G(d,p) level of theory.

File Name: Supplementary Dataset 3

Description: Supplementary Dataset 3 contains geometries in Cartesian coordinates in Å of different orientations of (M)-[123]tetramantane (Olympic rings, triangle and rhombus, 1a, 1b and 1c, respectively) computed using the GFN-xTB approach that were modelled on a Cu(111) slab consisting of 216 copper atoms at 15 K.