Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information for:

Size-dependent phase stability in transition metal dichalcogenide nanoparticles controlled by metal substrates

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This supplementary information document contains 5 figures (S1, S2, S3, S4 and S5).

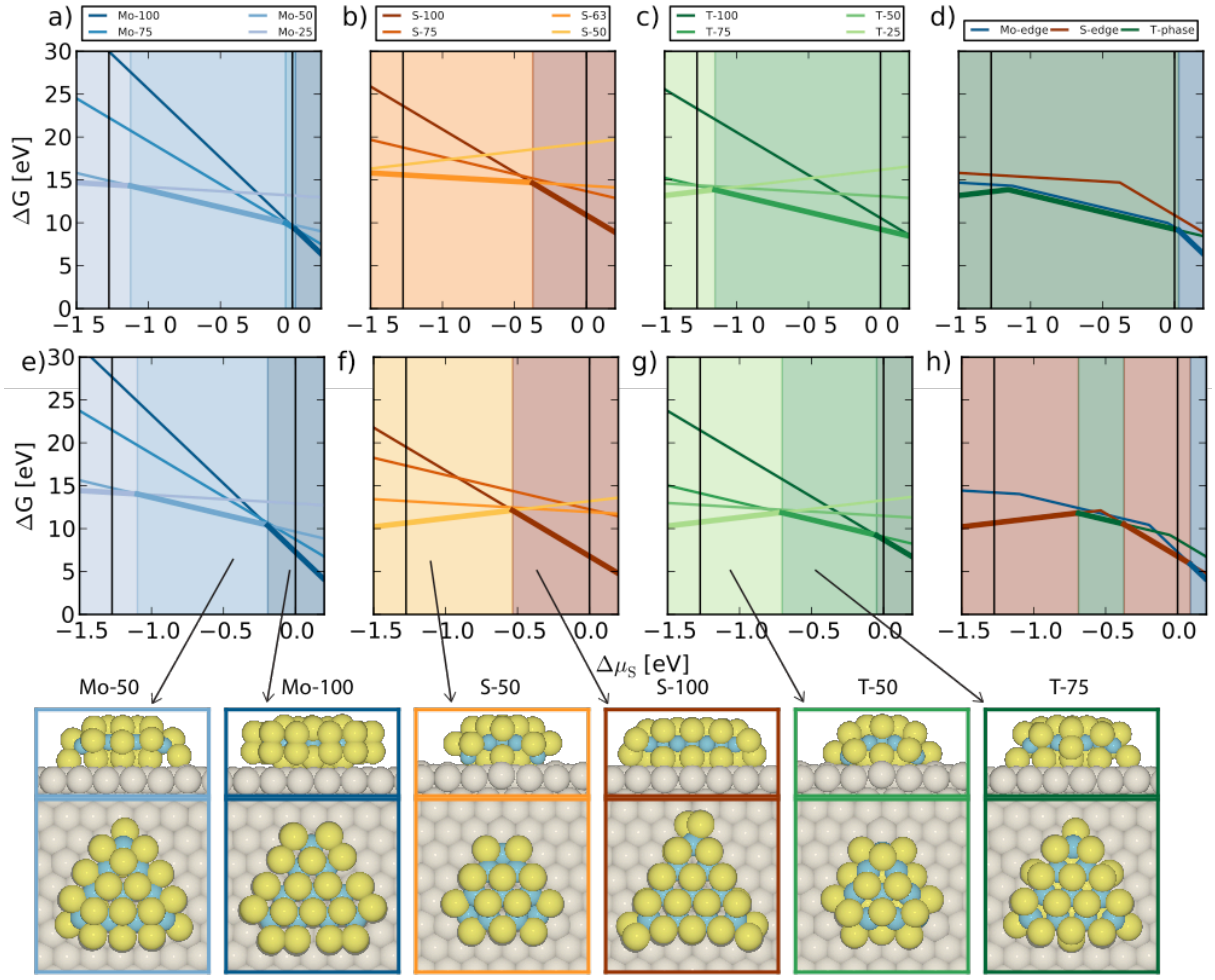

Figure S1: Phase diagrams for free-standing (a-d) and Au(111)-supported (e-h) MoS_2 NPs of size n=4 resulting from the *ab initio* thermodynamics analysis of the optimized structures. Blue, yellow, and grey spheres correspond to Mo, S, and Au atoms, respectively.

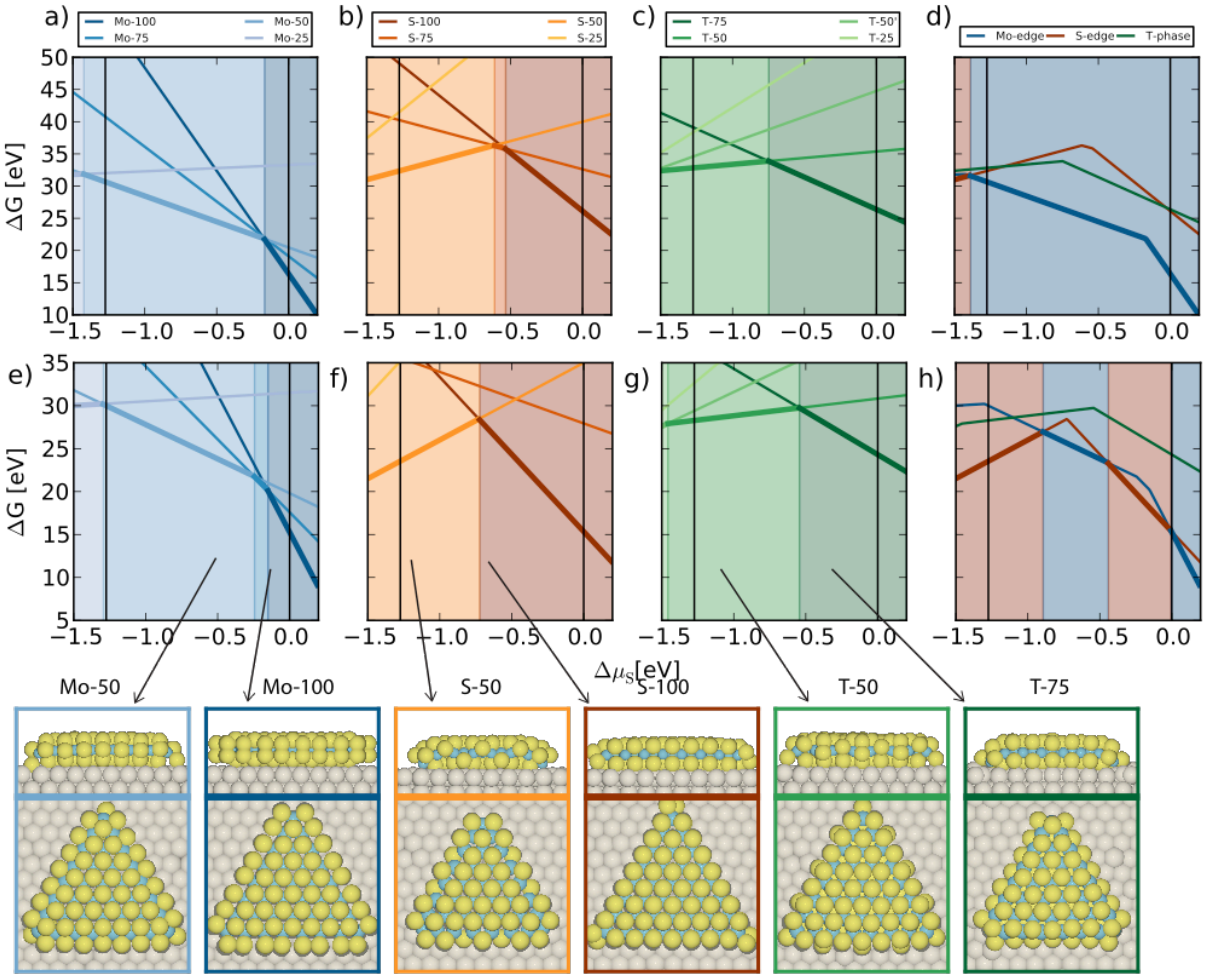

Figure S2: Phase diagrams for free-standing (a-d) and Au(111)-supported (e-h) MoS_2 NPs of size n=8 resulting from the *ab initio* thermodynamics analysis of the optimized structures. Blue, yellow, and grey spheres correspond to Mo, S, and Au atoms, respectively.

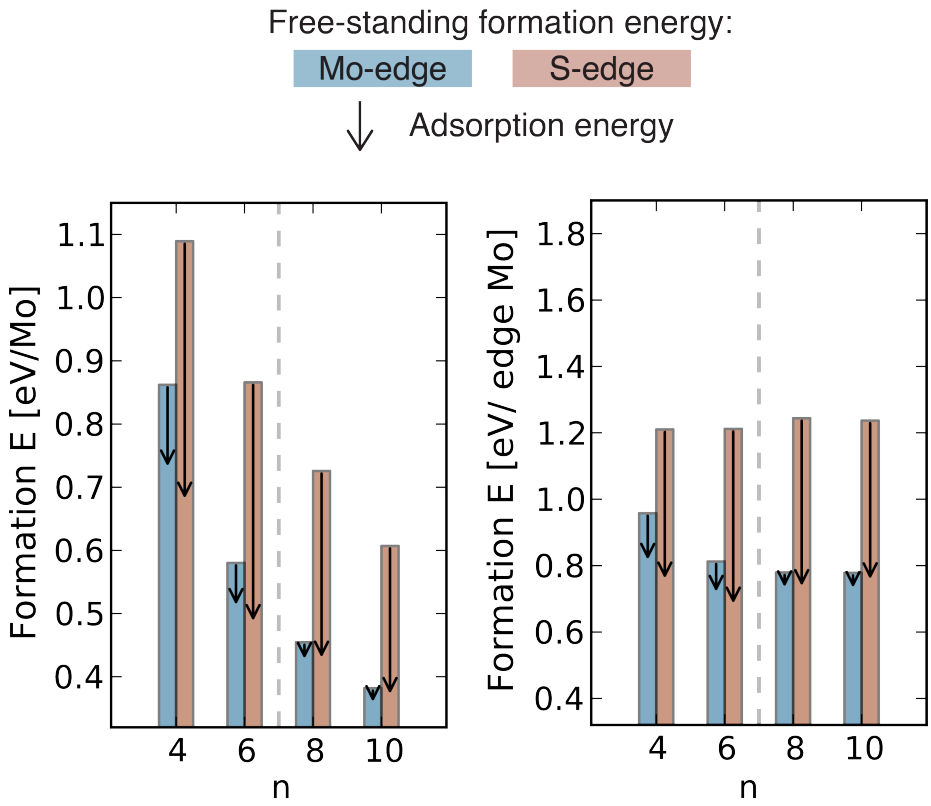

Figure S3: Formation energies of the freestanding Mo-100 (blue bars) and S-100 (red bars) MoS_2 NPs, with the corresponding adhesion energy on Au(111) indicated by the vertical black arrows. These quantities are normalized with respect to the total number of Mo atoms (left) and with respect to the total number of *edge* Mo atoms (right).

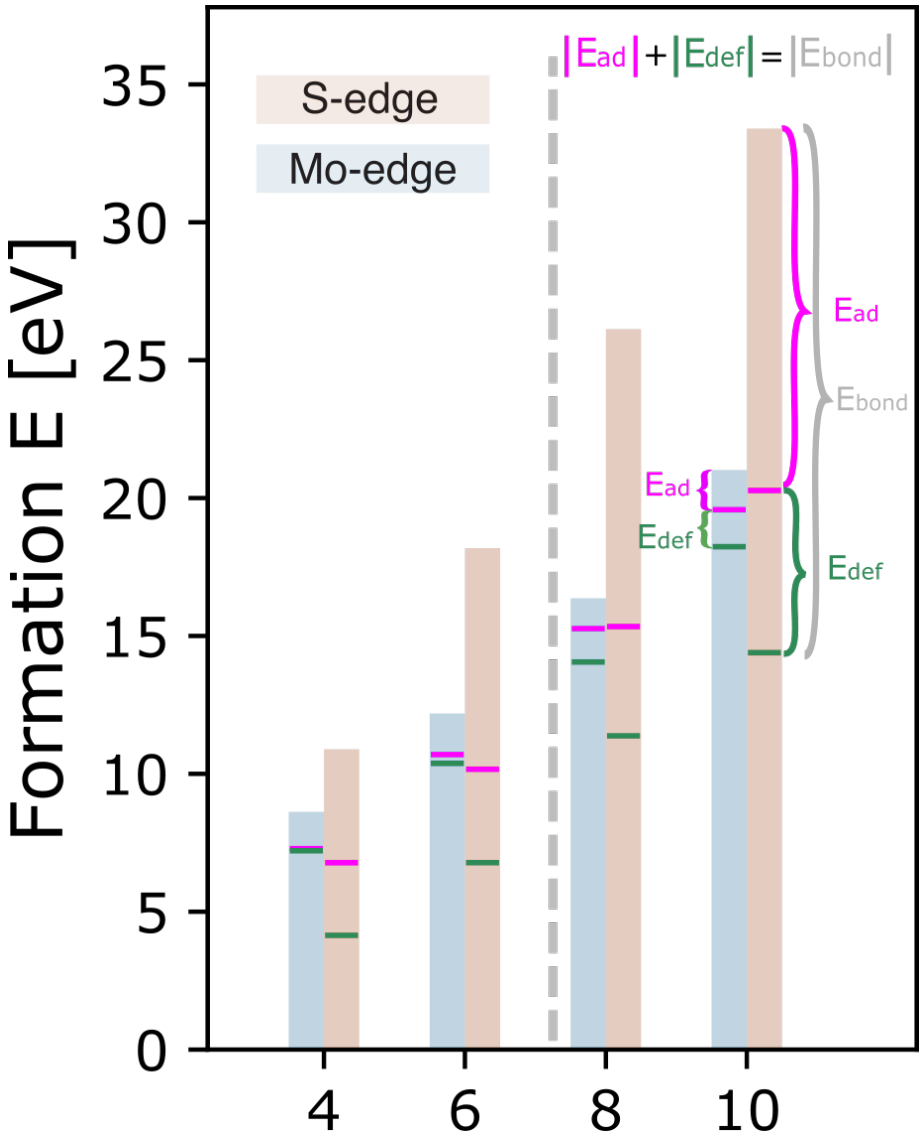

Figure S4: Formation energies of the freestanding Mo-100 (blue bars) and S-100 (red bars) MoS_2 NPs, with the corresponding adhesion energy on Au(111), and the deformation energy associated with that adhesion. In contrast to the images shown in Figures 4, 5, and S3, these formation energies have not been normalized by the number of Mo atoms of the nanoparticles, which allows for a better assessment of the different contributions to the formation energy of Au(111)-supported MoS_2 NPs. Note that the formation energy of the Au(111) supported energies corresponds to the fuchsia lines, whereas the green lines indicate the strength of the interaction between MoS_2 NPs and Au(111) without the deformation energy penalty.

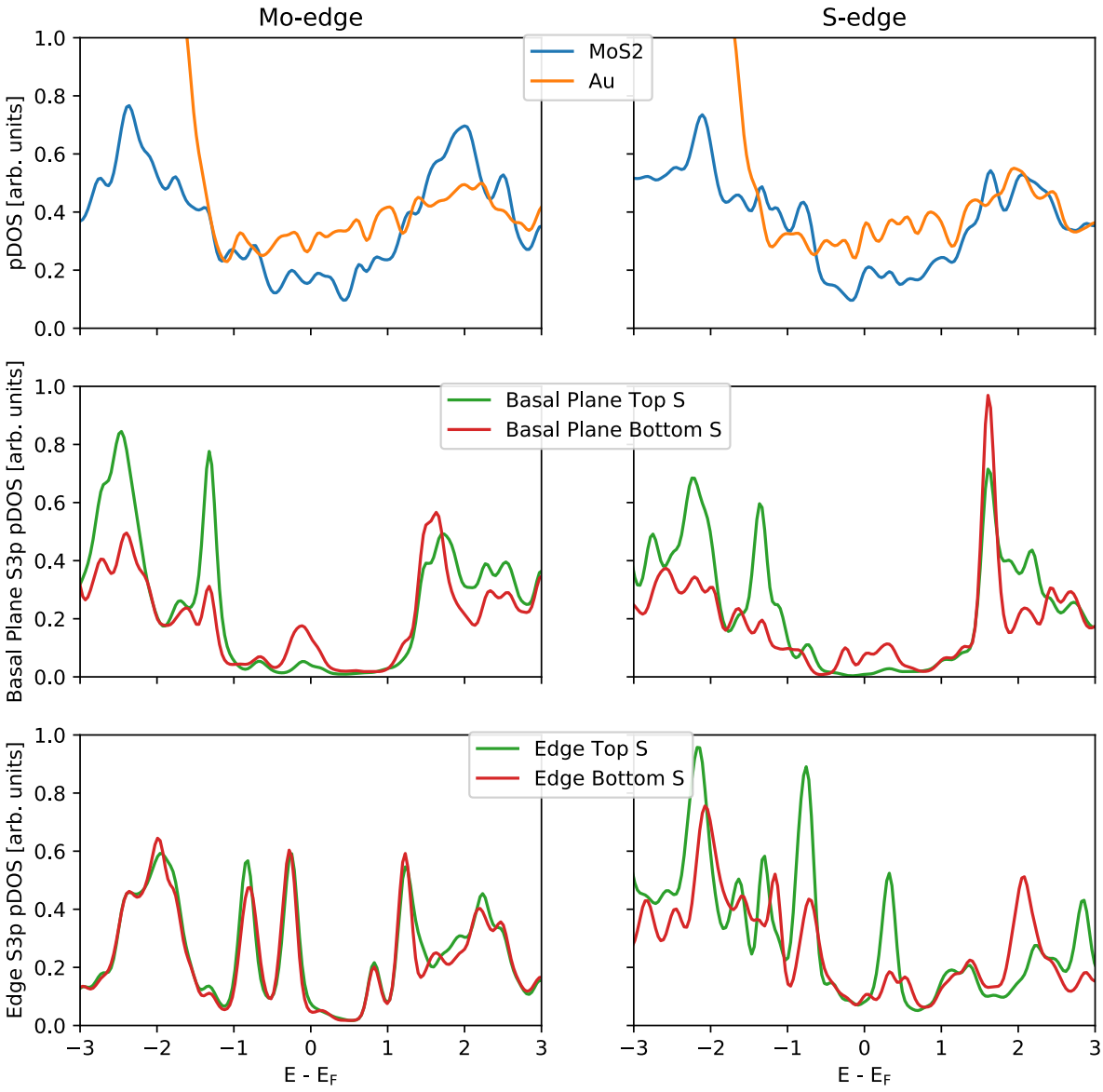

Figure S5: Projected density of states (pDOS) for Mo-100 and S-100 MoS_2 nanoparticles of size n = 6 supported on Au(111). Plots in the top row show pDOS projected onto the MoS_2 NP and Au(111) surface. Middle row plots show pDOS projected on basal plane S atoms from the top and bottom S layers. Bottom row plots show pDOS projected on edge S atoms from the top and bottom S layers.