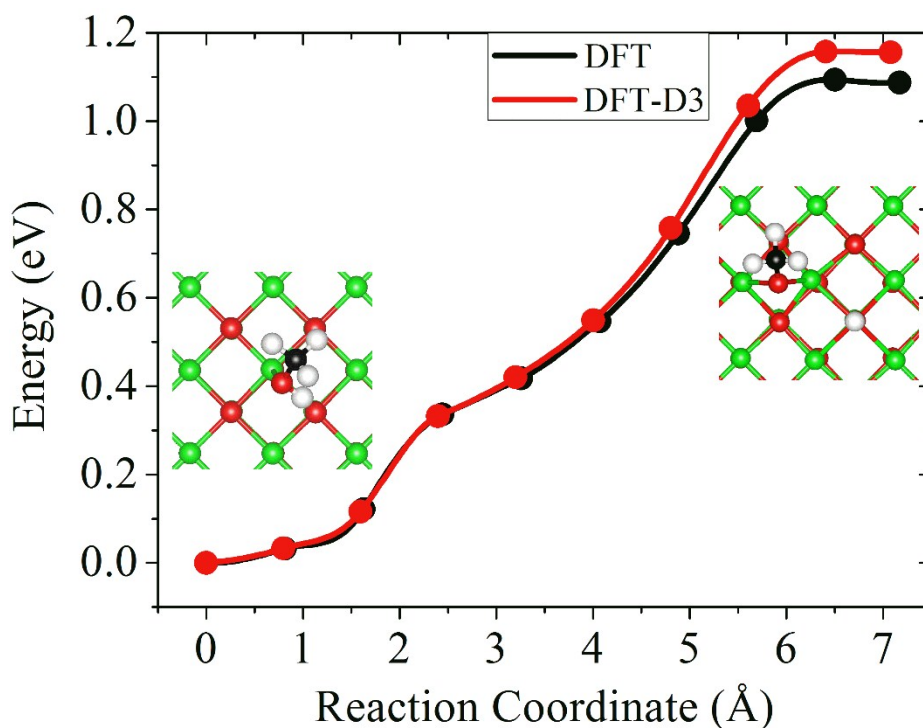# Splitting methanol on ultra-thin MgO(100) films deposited on a Mo substrate

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Figure S1. Potential energy profiles for the dissociation pathway of methanol (A → D) on the stoichiometric MgO(100) surface at DFT and DFT-D3 theoretical levels.

Table S1. Calculated bond lengths and surface rumplings of the *n* MgO layer of methanol adsorbed onto the MgO(100) at DFT-D3 level. All units are set in Å.

	Bond length		Bond length	Layer n	Δz_n[a]
C–Om	1.43	Mgs–O1	2.24	1	0.138
Om–H1	1.01	Mgs–O2	2.15	2	0.042
Om–Mgs	2.18	Mgs–O3	2.08	3	0.014
H1···O1	1.72	Mgs–O4	2.13	4	0.014
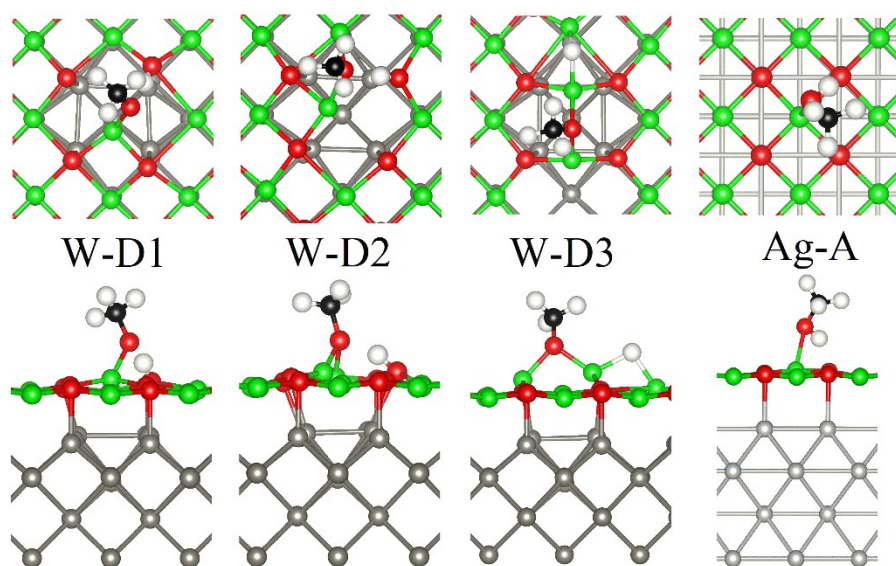
Figure S2. The adsorption geometries of methanol on the 1 ML MgO(100)/W(100) in the dissociative adsorption states (W-D1, W-D2 and W-D3) and the adsorption of methanol on the 1 MgO(100)/Ag(100) in the molecular form (Ag-A).