C–H Bond Activation of Methane via σ–d Interaction on the IrO_2(110) Surface: Density Functional Theory Study

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Supporting Information

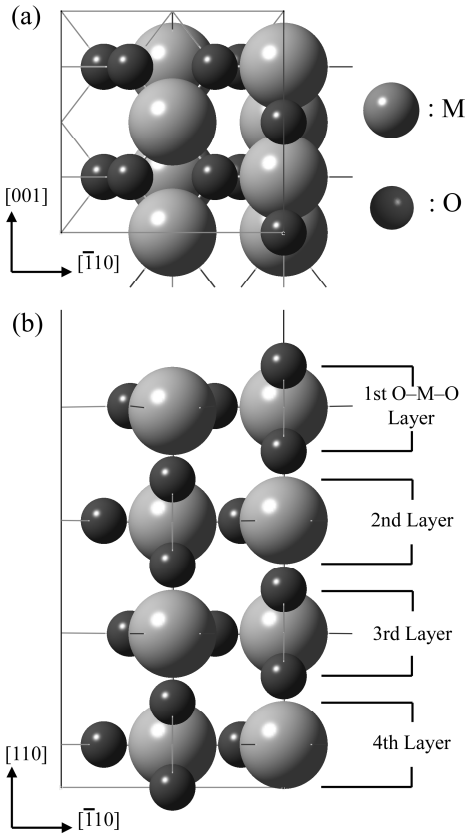

Figure S1. (a) Top and (b) side views and layer definition of the MO_2(110) (M = Ir, Ru or Ti) surface models applied in this work.

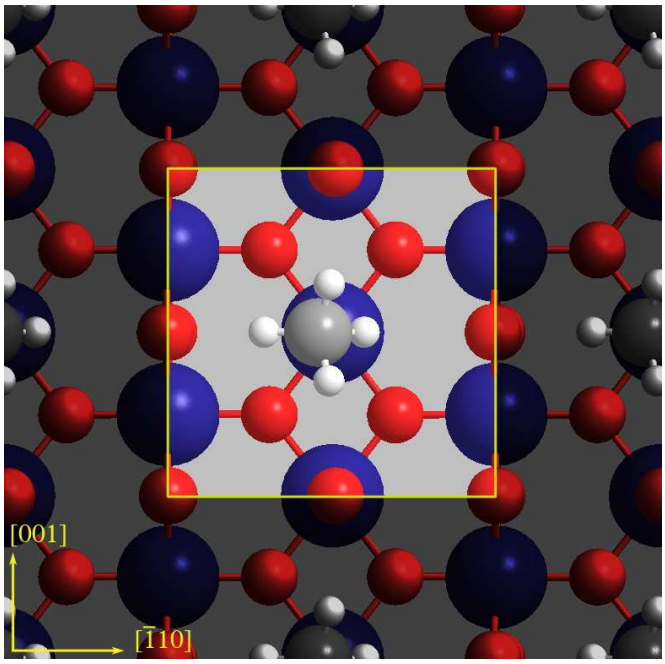

Figure S2. The top view of methane adsorption on the oxygen-rich IrO_2(110) surface. The central rectangular demonstrates the 2 × 1 supercell.

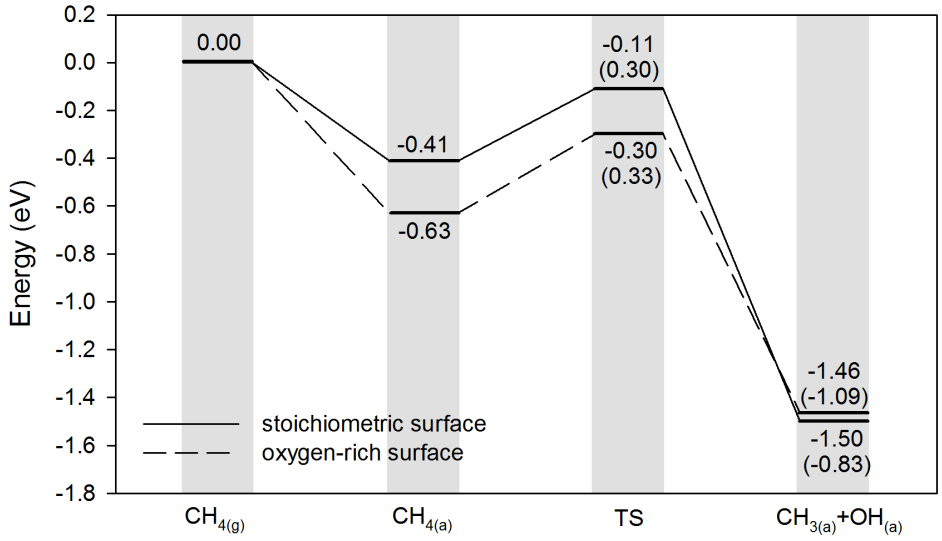

Figure S3. The potential energy surface of methane adsorption and the hydrogen atom abstraction reaction on $IrO_2(110)$ surfaces.

TABLE S1: Selected Geometric Parameters (Å) of Transition State and Final State of Hydrogen Atom Abstraction by the Stoichiometric $IrO_2(110)$ Surface

	Transition State	Final State
$d(C–H_a)$	1.11	1.10
$d(C–H_b)$	1.40	2.36
$d(C–H_c)$	1.11	1.11
$d(O_{br}–H_b)$	1.28	0.98
$d(Ir_{cus}–C)$	2.26	2.07