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Supplementary Information

Selectivity for Ethanol Partial Oxidation: The Unique Chemistry of Single-Atom Alloy Catalysts on Au, Ag, and Cu(111)

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Table S1. Convergence test on the slab thickness of a $Pd_1/Cu(111)$ surface.

	EtOH-Binding	**H-Binding**	**O-Binding**	**OH-Binding**	**CO-Binding**
3-Layer	**-0.71 eV**	**-2.69 eV**	**-5.04 eV**	**-3.32 eV**	**-1.97 eV**
5-Layer	**-0.72 eV**	**-2.69 eV**	**-4.97 eV**	**-3.29 eV**	**-2.00 eV**
Relative Error	**1.39%**	**0.00%**	**1.41%**	**0.91%**	**1.50%**

Note: All the binding energies were calculated using the total energies of a bare slab and the adsorbate in vacuum as references. The adsorbate total energies were calculated with spin-polarization.

Table S2. Reaction energy of a dopant leaching out from the (111) surface (E_{Leach}). Schematic pictures can be found in **Figure S1**.

Surfaces	E_{Leach} (eV)
Cu_1/Au(111)	**1.55**
Ir_1/Au(111)	**2.72**
Pd_1/Au(111)	**1.71**
Pt_1/Au(111)	**2.01**
Rh_1/Au(111)	**2.35**
Cu_1/Ag(111)	**1.43**
Ir_1/Ag(111)	**2.84**
Pd_1/Ag(111)	**1.79**
Pt_1/Ag(111)	**2.10**
Rh_1/Ag(111)	**2.50**
Ir_1/Cu(111)	**3.37**
Pd_1/Cu(111)	**2.05**
Pt_1/Cu(111)	**2.50**
Rh_1/Cu(111)	**2.89**

Table S3. Reaction energies of two surface isolated dopants forming a dimer (E_{Dimer}). Schematic picture can be found in **Figure S1**.

Surfaces	E_{Dimer} (eV)
Cu_1/Au(111)	**0.09**
Ir_1/Au(111)	**-0.25**
Pd_1/Au(111)	**0.07**
Pt_1/Au(111)	**-0.01**
Rh_1/Au(111)	**0.02**
Cu_1/Ag(111)	**0.03**
Ir_1/Ag(111)	**-0.38**
Pd_1/Ag(111)	**0.05**
Pt_1/Ag(111)	**-0.05**
Rh_1/Ag(111)	**-0.05**
Ir_1/Cu(111)	**-0.06**
Pd_1/Cu(111)	**0.11**
Pt_1/Cu(111)	**0.11**
Rh_1/Cu(111)	**0.07**

Table S4. Calculated binding energy of EtOH (E_b), activation energy barrier (E_{act}), and reaction energy (E_{react}) on the studied fourteen single-atom alloy surfaces.

Surfaces	E_b [EtOH] (eV)	E_{act} [O-H] (eV)	E_{react} [O-H] (eV)	E_{act} [α-C-H] (eV)	E_{react} [α-C-H] (eV)	E_{act} [β -C-H] (eV)	E_{react} [β -C-H] (eV)
Cu_1/Au(111)	**-0.85**	**1.27**	**1.24**	**1.55**	**1.42**	**1.66**	**1.12**
Ir_1/Au(111)	**-0.95**	**1.29**	**0.94**	**0.68**	**0.18**	**1.67**	**1.10**
Pd_1/Au(111)	**-0.67**	**1.55**	**1.88**	**0.82**	**0.82**	**1.66**	**1.11**
Pt_1/Au(111)	**-0.66**	**1.16**	**1.05**	**0.84**	**0.37**	**1.66**	**1.12**
Rh_1/Au(111)	**-0.91**	**1.21**	**0.97**	**0.55**	**0.47**	**1.70**	**1.12**
Cu_1/Ag(111)	**-0.65**	**1.13**	**0.37**	**1.48**	**1.13**	**1.66**	**1.31**
Ir_1/Ag(111)	**-0.75**	**0.77**	**-0.04**	**0.51**	**-0.16**	**1.67**	**1.30**
Pd_1/Ag(111)	**-0.55**	**1.35**	**0.69**	**0.92**	**0.81**	**1.66**	**1.43**
Pt_1/Ag(111)	**-0.46**	**0.84**	**0.57**	**0.79**	**0.25**	**1.56**	**1.00**
Rh_1/Ag(111)	**-0.75**	**0.75**	**0.20**	**0.60**	**0.27**	**1.63**	**1.37**
Ir_1/Cu(111)	**-0.85**	**0.93**	**-0.00**	**0.66**	**-0.03**	**1.39**	**1.05**
Pd_1/Cu(111)	**-0.71**	**1.42**	**-0.00**	**1.13**	**0.51**	**1.45**	**0.76**
Pt_1/Cu(111)	**-0.64**	**2.00**	**0.84**	**0.77**	**0.15**	**1.18**	**0.70**
Rh_1/Cu(111)	**-0.87**	**1.06**	**0.00**	**0.42**	**0.24**	**1.33**	**1.05**

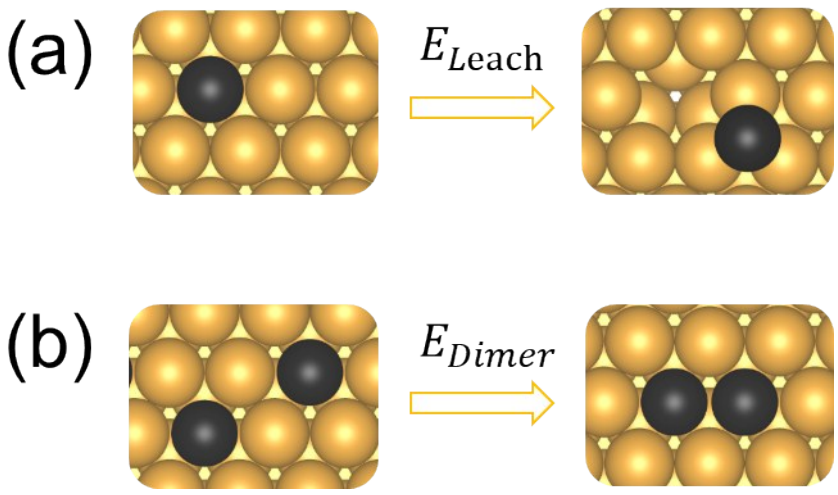

Figure S1. Schematic pictures of (a) a dopant leaching out from the (111) surface and (b) two surface isolated dopants forming a dimer.

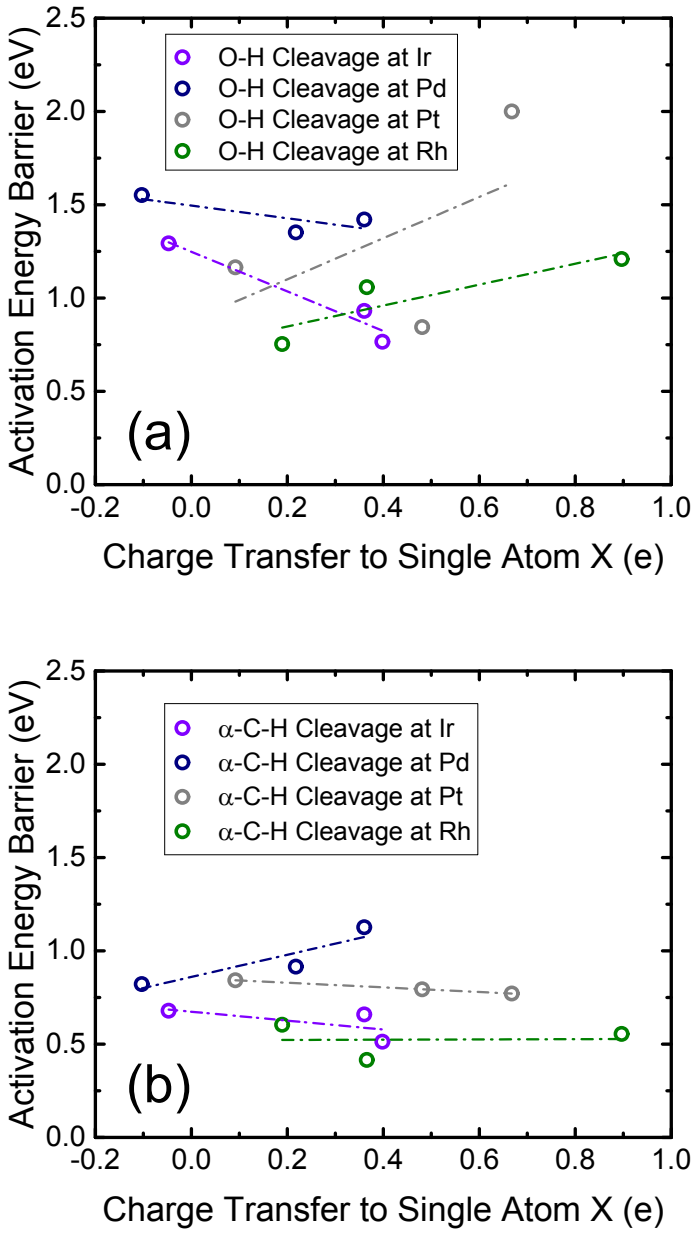

Figure S2. Correlation between (a) O-H activation energy and charge transfer effect and (b) α-C-H activation energy and charge transfer effect.