ЖУРНАЛ СТРУКТУРНОЙ ХИМИИ

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SUPPLEMENTARY MATERIALS TO:

Re- AND Cs-COPROMOTED SILVER CATALYSTS FOR ETHYLENE EPOXIDATION: A THEORETICAL STUDY

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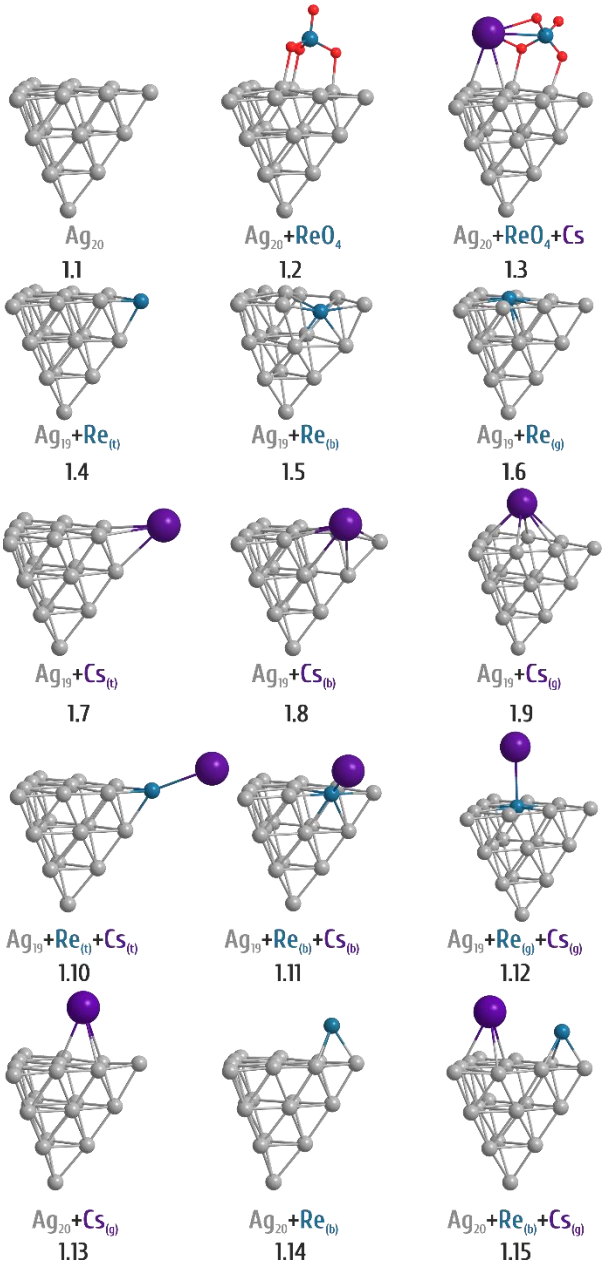

Fig. S1. A selection of developed cluster models. Gray, red, dark cyan, and royal colors correspond to silver, oxygen, rhenium, and cesium atoms, respectively.

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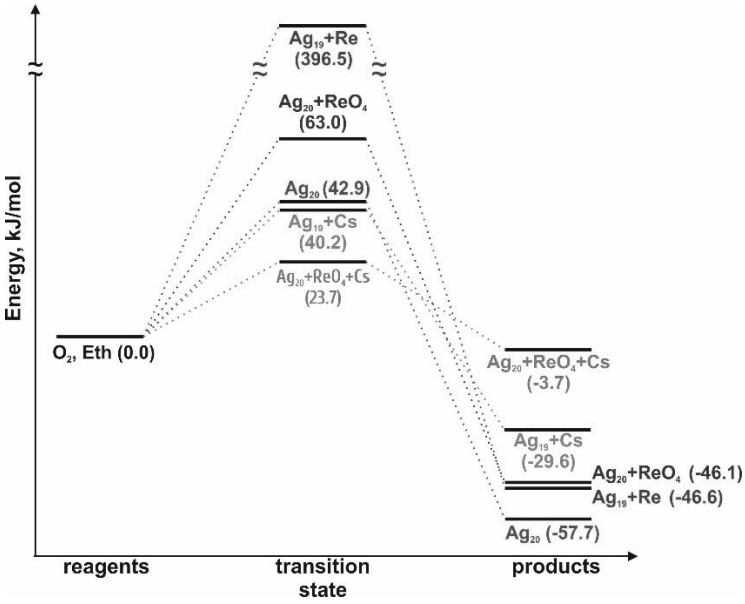

Fig. S2. Reaction energy diagrams for selected models. The values in parentheses show energy barriers (kJ/mol) to corresponding transition states (positive values) and reaction products (negative values).

Table S1

Optimized geometry parameters for transition state structures over the developed models

System	C–C	C–H*	C–O	Ag–O	Re–O*	Cs–O*	Ag–C
Oxametallacycle formation							
Ag_{20}+$OMC_{(b)}$_TS	1.518	1.103	1.392	2.346	–	–	2.264
Ag_{19}+Cs+$OMC_{(b)}$_TS	1.523	1.108	1.375	2.274	–	2.974	2.248
Ag_{20}+$ReO_{4(t)}$+$OMC_{(b)}$_TS	1.491	1.093	1.441	2.188, 2.560 to ReO_4 2.327	1.761	–	2.791
Ag_{20}+$ReO_{4(b)}$+$Cs_{(b)}$+$OMC_{(b)}$_TS	1.523	1.105	1.398	2.502 to ReO_4 2.493	1.748	to ReO_4 3.199 to O atom 3.163	2.298

* Mean values, Å

Table S2

Binding energies (kJ/mol) *for* O_2 *and ethylene adsorption,* O *chemisorption, and formation of* EO OMC. *The results obtained at* B3LYP/Lanl2DZ *level of theory*

Process/Model	Ag_{20}	Ag_{19}+Cs	Ag_{19}+Re	Ag_{19}+Re+Cs	Ag_{20}+ReO_4	Ag_{20}+ReO_4+Cs
			O_2 adsorption			
Terminal	–54	–166	–354	–435	–37	+2
Bridge	–26	–218	–348	–286	–32	–100
Grain	+33	–118	–357	–309	–35	–95
			O chemisorption			
Terminal	–514	–541	–555	–621	–566	–568
Bridge	–550	–542	–566	–649	–569	–582
Grain	–550	–559	–552	–598	–565	–567
			Ethylene adsorption			
Terminal	–18	–14	–227	–59	–12	–18
Bridge	–5	–14	–158	–131	–14	–30
Grain	–3	–14	–192	–4	–13	–24
			OMC formation			
Terminal	–193	–288	–275	–270	–301	–282
Bridge	–264	–313	–689	–116	–307	–297
Grain	–236	–312	–581	–157	–269	–282

Table S3

Mulliken charge over Re, Cs, Ag *and* O *atoms*

System	Re	Cs	O
Ag_{20}+$OMC_{(b)}$	–	–	–0.567
Ag_{19}+$Re_{(t)}$+$OMC_{(b)}$	–0.138	–	–0.580
Ag_{19}+$Cs_{(b)}$+$OMC_{(b)}$	–	+0.936	–0.655
Ag_{20}+$Re_{(t)}$+$OMC_{(b)}$	–0.211	–	–0.544
Ag_{20}+Cs+$OMC_{(b)}$	–	+0.932	–0.600
Ag_{19}+$Re_{(b)}$+$Cs_{(g)}$+$OMC_{(b)}$	–0.174	+0.888	–0.644
Ag_{20}+$Re_{(t)}$+$Cs_{(t)}$+$OMC_{(b)}$	–0.246	+0.787	–0.553
Ag_{20}+$ReO_{4(t)}$+$OMC_{(b)}$	+2.123	–	–0.568
Ag_{20}+$ReO_{4(b)}$+$Cs_{(b)}$+$OMC_{(b)}$	+2.059	+0.933	–0.552