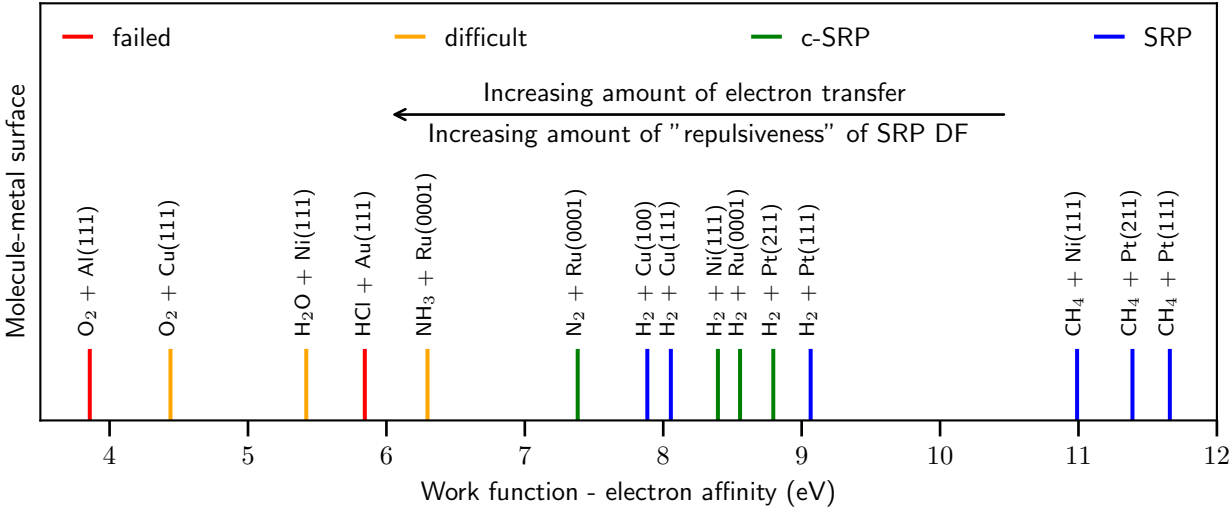
failed
difficult
c-SRP
SRP
Increasing amount of electron transfer
Increasing amount of "repulsiveness" of SRP DF
Molecule-metal surface
O2 + Al(111)
O2 + Cu(111)
H2O + Ni(111)
HCl + Au(111)
NH3 + Ru(0001)
N2 + Ru(0001)
H2 + Cu(100)
H2 + Cu(111)
H2 + Ni(111)
H2 + Ru(0001)
H2 + Pt(211)
H2 + Pt(111)
CH4 + Ni(111)
CH4 + Pt(211)
CH4 + Pt(111)
4
5
6
7
8
9
10
11
12
Work function - electron affinity (eV)