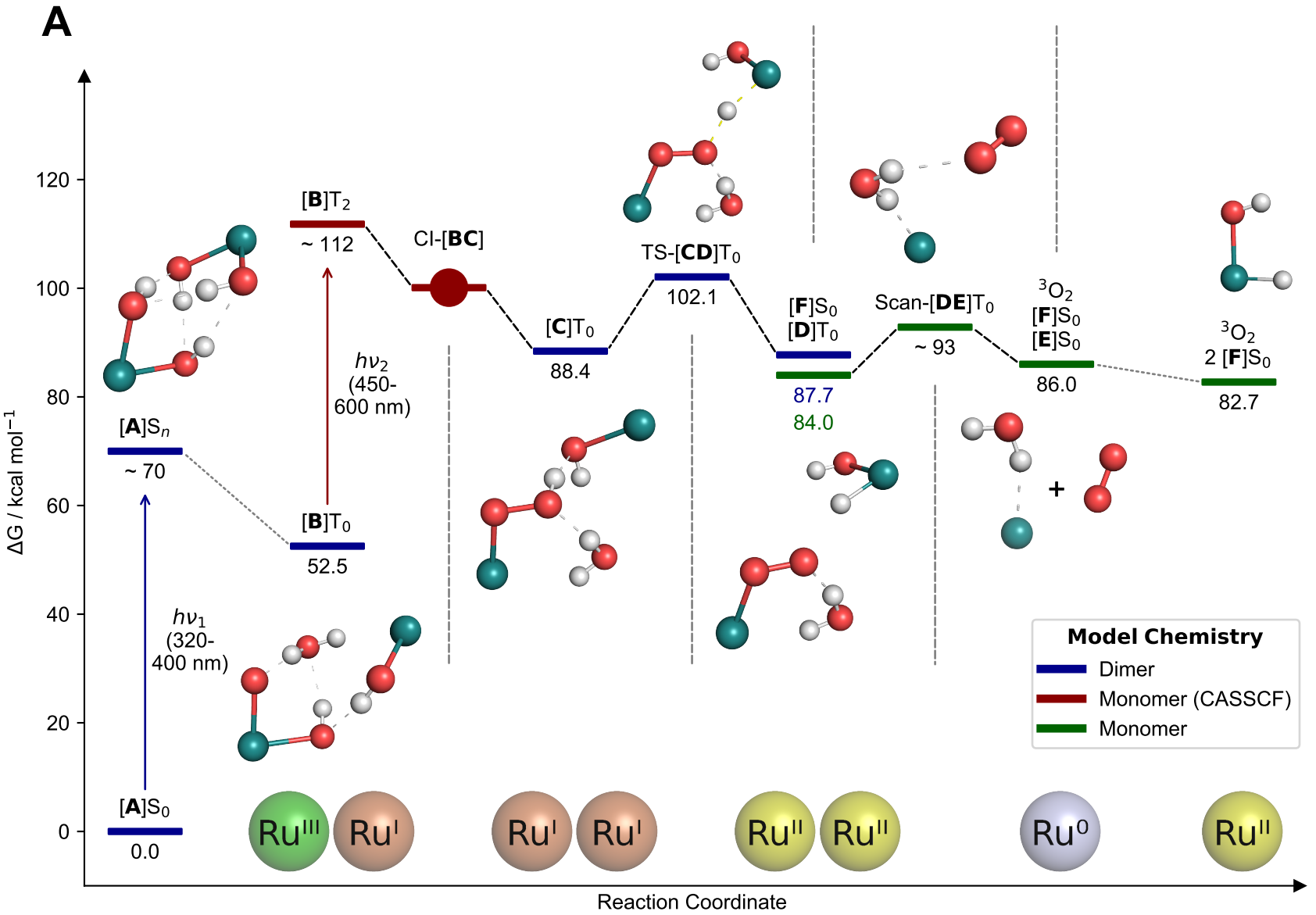
A
ΔG / kcal mol⁻¹
120
100
80
60
40
20
0
[A]Sn
~ 70
[A]S0
0.0
hν1
(320-
400 nm)
[B]T2
~ 112
hν2
(450-
600 nm)
[B]T0
52.5
CI-[BC]
[C]T0
88.4
TS-[CD]T0
102.1
[F]S0
[D]T0
87.7
84.0
Scan-[DE]T0
~ 93
3O2
[F]S0
[E]S0
86.0
3O2
2 [F]S0
82.7
+
Ru^III
Ru^I
Ru^I
Ru^I
Ru^II
Ru^II
Ru^0
Ru^II
Model Chemistry
Dimer
Monomer (CASSCF)
Monomer
Reaction Coordinate