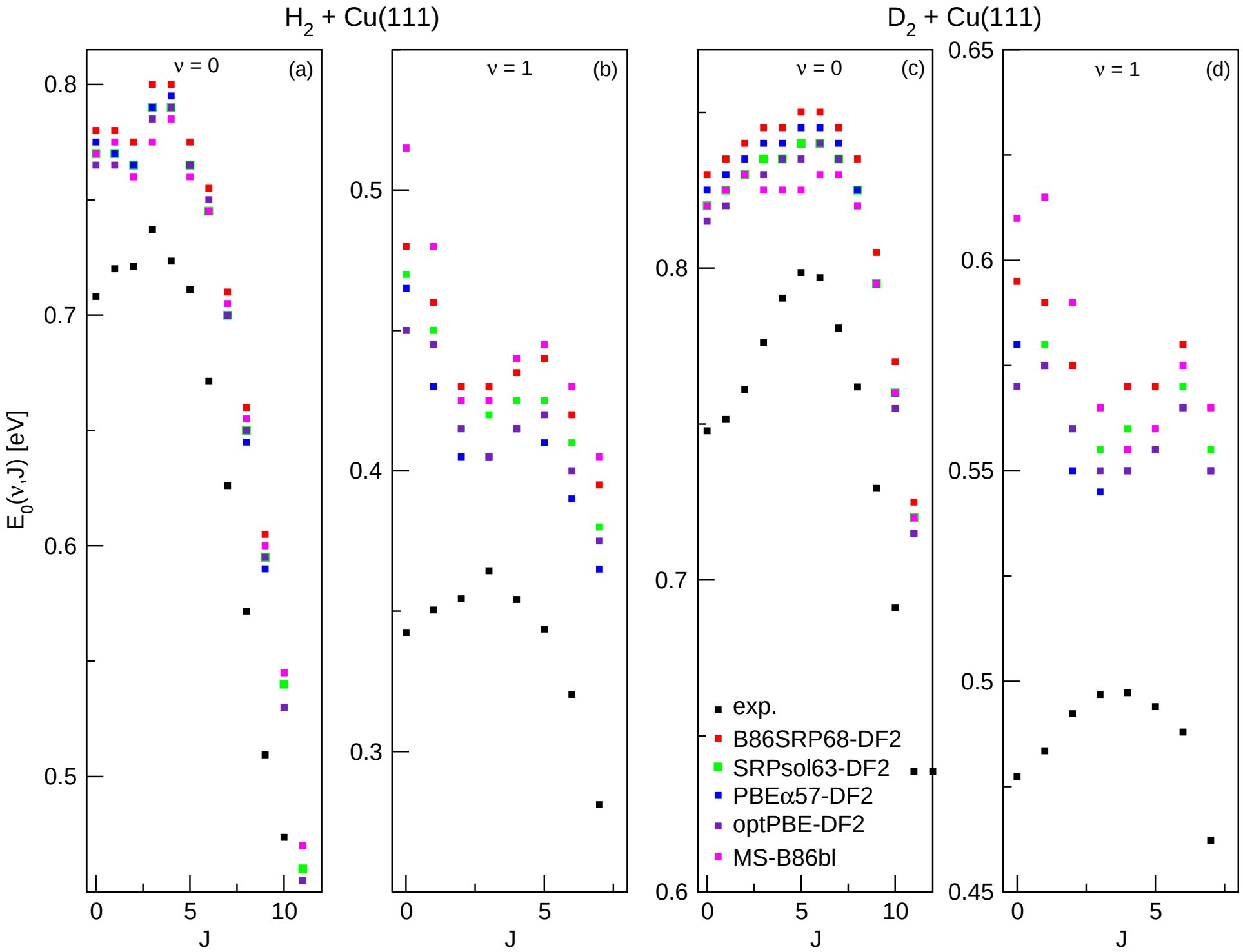
H2 + Cu(111)
D2 + Cu(111)
ν = 0
(a)
ν = 1
(b)
ν = 0
(c)
ν = 1
(d)
E0(ν,J) [eV]
J
exp.
B86SRP68-DF2
SRPsol63-DF2
PBEα57-DF2
optPBE-DF2
MS-B86bl