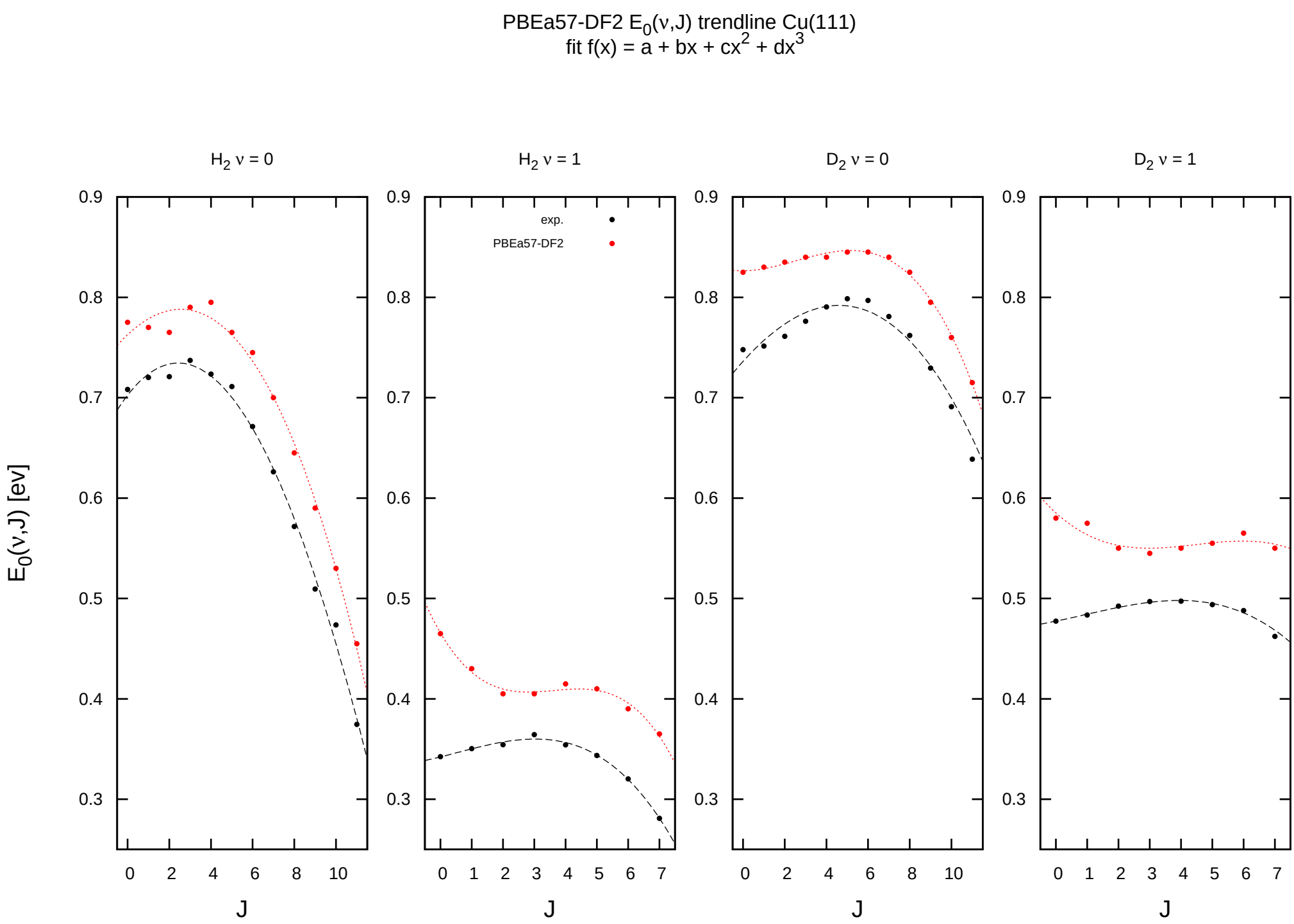
PBEa57-DF2 E0(ν,J) trendline Cu(111)
fit f(x) = a + bx + cx2 + dx3
H2 ν = 0
H2 ν = 1
D2 ν = 0
D2 ν = 1
exp.
PBEa57-DF2
E0(ν,J) [ev]
J
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0 2 4 6 8 10
0 1 2 3 4 5 6 7