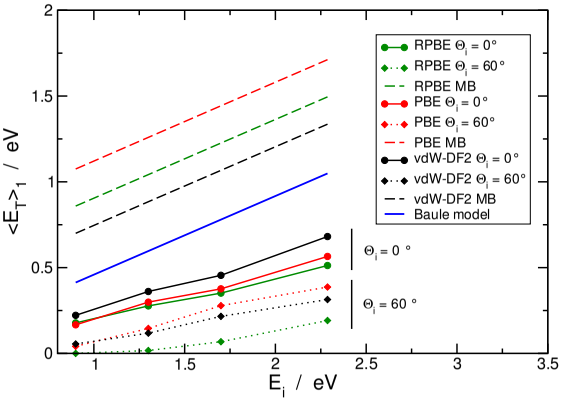
RPBE Θi = 0°
RPBE Θi = 60°
RPBE MB
PBE Θi = 0°
PBE Θi = 60°
PBE MB
vdW-DF2 Θi = 0°
vdW-DF2 Θi = 60°
vdW-DF2 MB
Baule model
Θi = 0 °
Θi = 60 °
<ET>1 / eV
Ei / eV
0
0.5
1
1.5
2
1
1.5
2
2.5
3
3.5