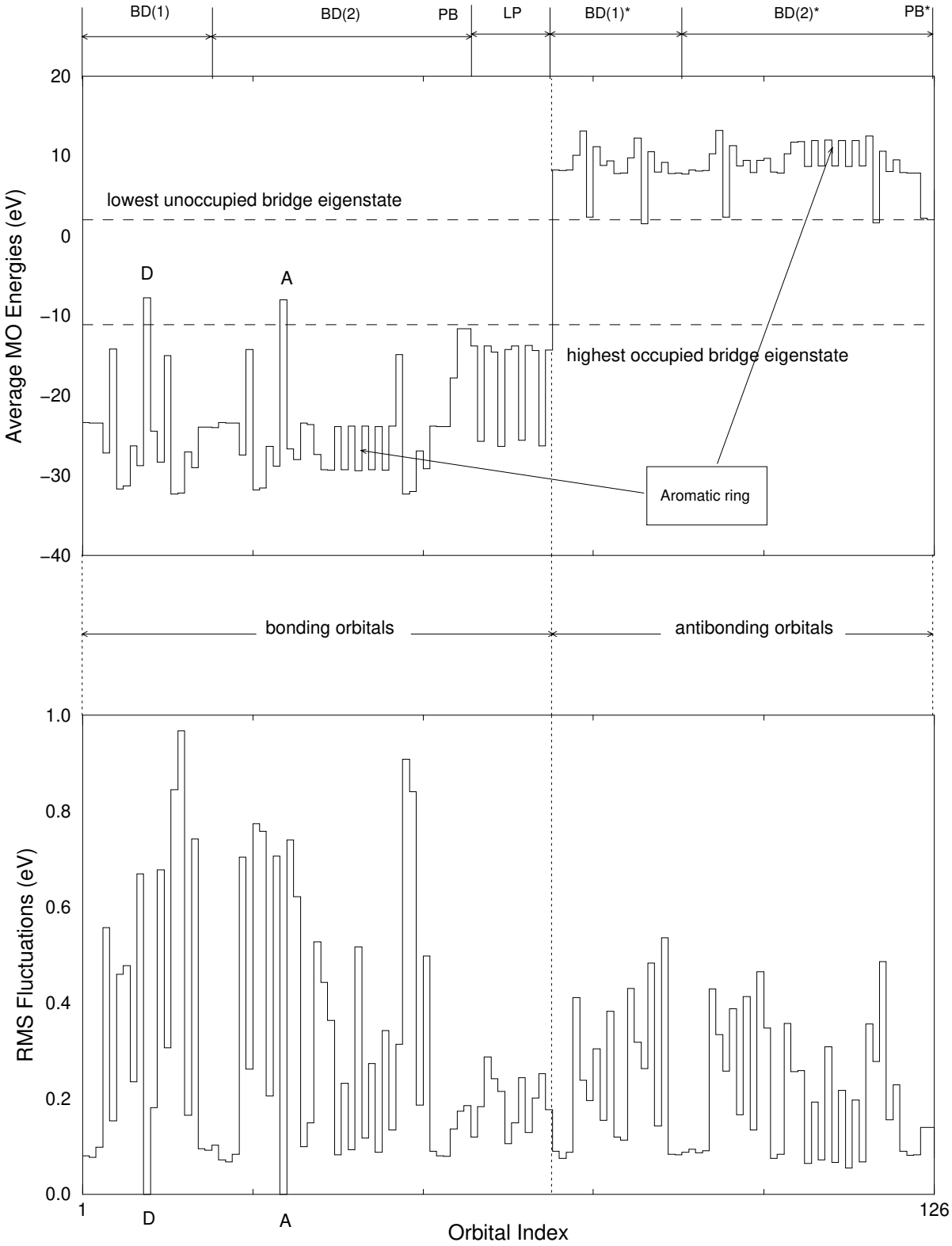
BD(1)
BD(2)
PB
LP
BD(1)*
BD(2)*
PB*
20
10
0
−10
−20
−30
−40
Average MO Energies (eV)
lowest unoccupied bridge eigenstate
highest occupied bridge eigenstate
D
A
Aromatic ring
bonding orbitals
antibonding orbitals
1.0
0.8
0.6
0.4
0.2
0.0
RMS Fluctuations (eV)
1
D
A
126
Orbital Index