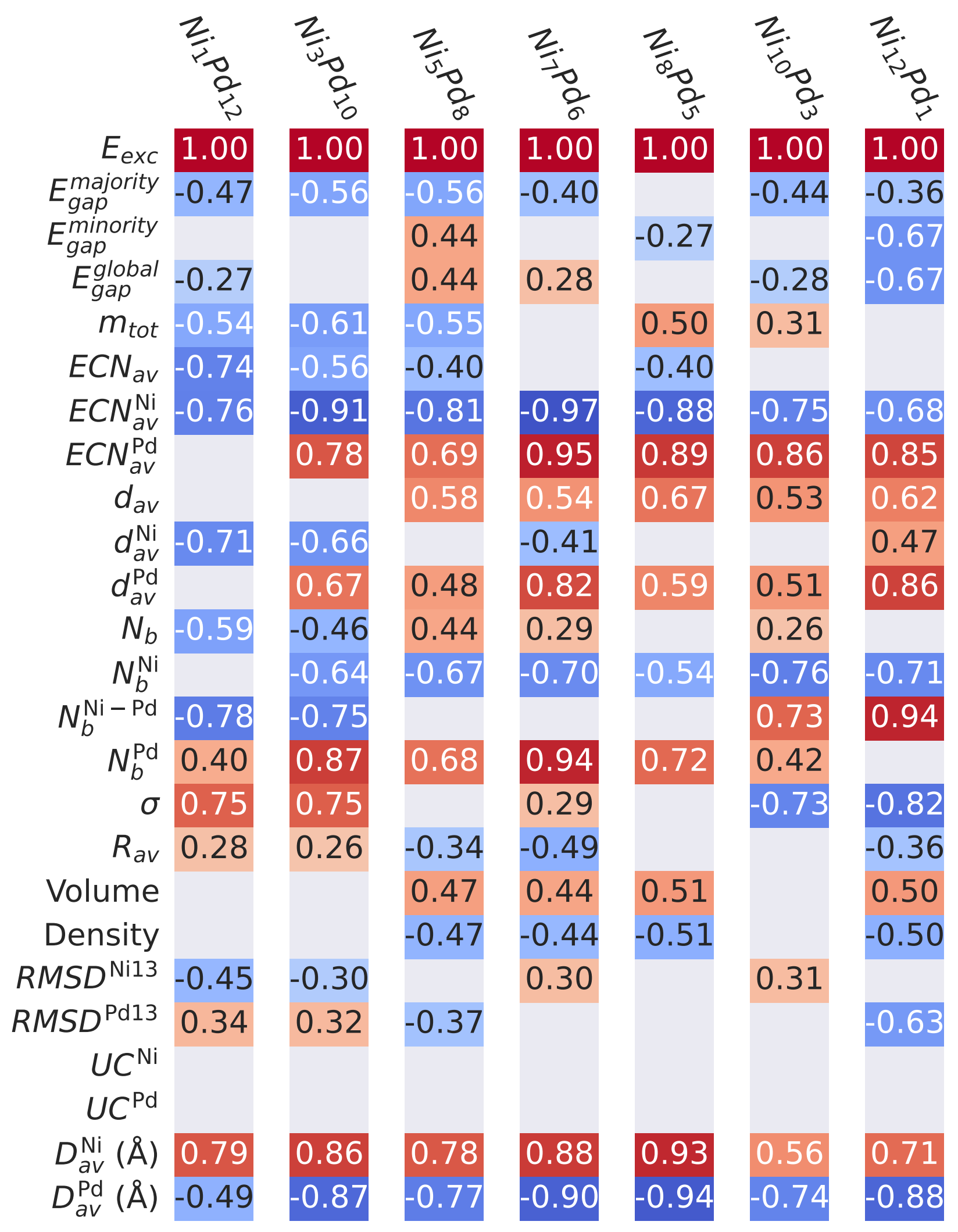
Ni_1Pd_{12}
Ni_3Pd_{10}
Ni_5Pd_8
Ni_7Pd_6
Ni_8Pd_5
$Ni_{10}Pd_3$
$Ni_{12}Pd_1$
E_{exc} 1.00 1.00 1.00 1.00 1.00 1.00 1.00
$E_{gap}^{majority}$ -0.47 -0.56 -0.56 -0.40 -0.44 -0.36
$E_{gap}^{minority}$ 0.44 -0.27 -0.67
E_{gap}^{global} -0.27 0.44 0.28 -0.28 -0.67
m_{tot} -0.54 -0.61 -0.55 0.50 0.31
ECN_{av} -0.74 -0.56 -0.40 -0.40
ECN_{av}^{Ni} -0.76 -0.91 -0.81 -0.97 -0.88 -0.75 -0.68
ECN_{av}^{Pd} 0.78 0.69 0.95 0.89 0.86 0.85
d_{av} 0.58 0.54 0.67 0.53 0.62
d_{av}^{Ni} -0.71 -0.66 -0.41 0.47
d_{av}^{Pd} 0.67 0.48 0.82 0.59 0.51 0.86
N_b -0.59 -0.46 0.44 0.29 0.26
N_b^{Ni} -0.64 -0.67 -0.70 -0.54 -0.76 -0.71
N_b^{Ni-Pd} -0.78 -0.75 0.73 0.94
N_b^{Pd} 0.40 0.87 0.68 0.94 0.72 0.42
σ 0.75 0.75 0.29 -0.73 -0.82
R_{av} 0.28 0.26 -0.34 -0.49 -0.36
Volume 0.47 0.44 0.51 0.50
Density -0.47 -0.44 -0.51 -0.50
$RMSD^{Ni13}$ -0.45 -0.30 0.30 0.31
$RMSD^{Pd13}$ 0.34 0.32 -0.37 -0.63
UC^{Ni}
UC^{Pd}
D_{av}^{Ni} (Å) 0.79 0.86 0.78 0.88 0.93 0.56 0.71
D_{av}^{Pd} (Å) -0.49 -0.87 -0.77 -0.90 -0.94 -0.74 -0.88