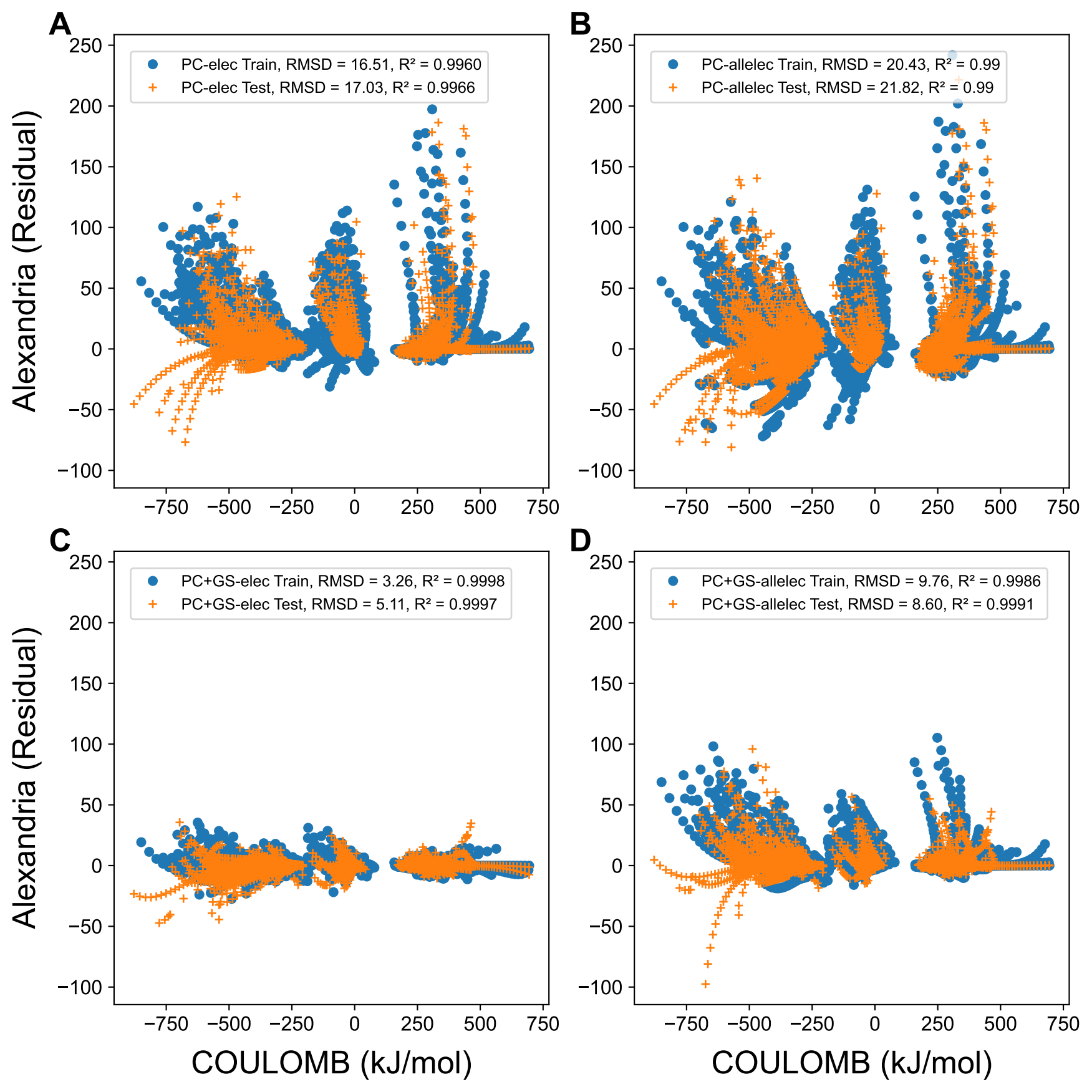
A
PC-elec Train, RMSD = 16.51, R² = 0.9960
PC-elec Test, RMSD = 17.03, R² = 0.9966
B
PC-allelec Train, RMSD = 20.43, R² = 0.99
PC-allelec Test, RMSD = 21.82, R² = 0.99
C
PC+GS-elec Train, RMSD = 3.26, R² = 0.9998
PC+GS-elec Test, RMSD = 5.11, R² = 0.9997
D
PC+GS-allelec Train, RMSD = 9.76, R² = 0.9986
PC+GS-allelec Test, RMSD = 8.60, R² = 0.9991
Alexandria (Residual)
COULOMB (kJ/mol)
250
200
150
100
50
0
−50
−100
−750
−500
−250
0
250
500
750