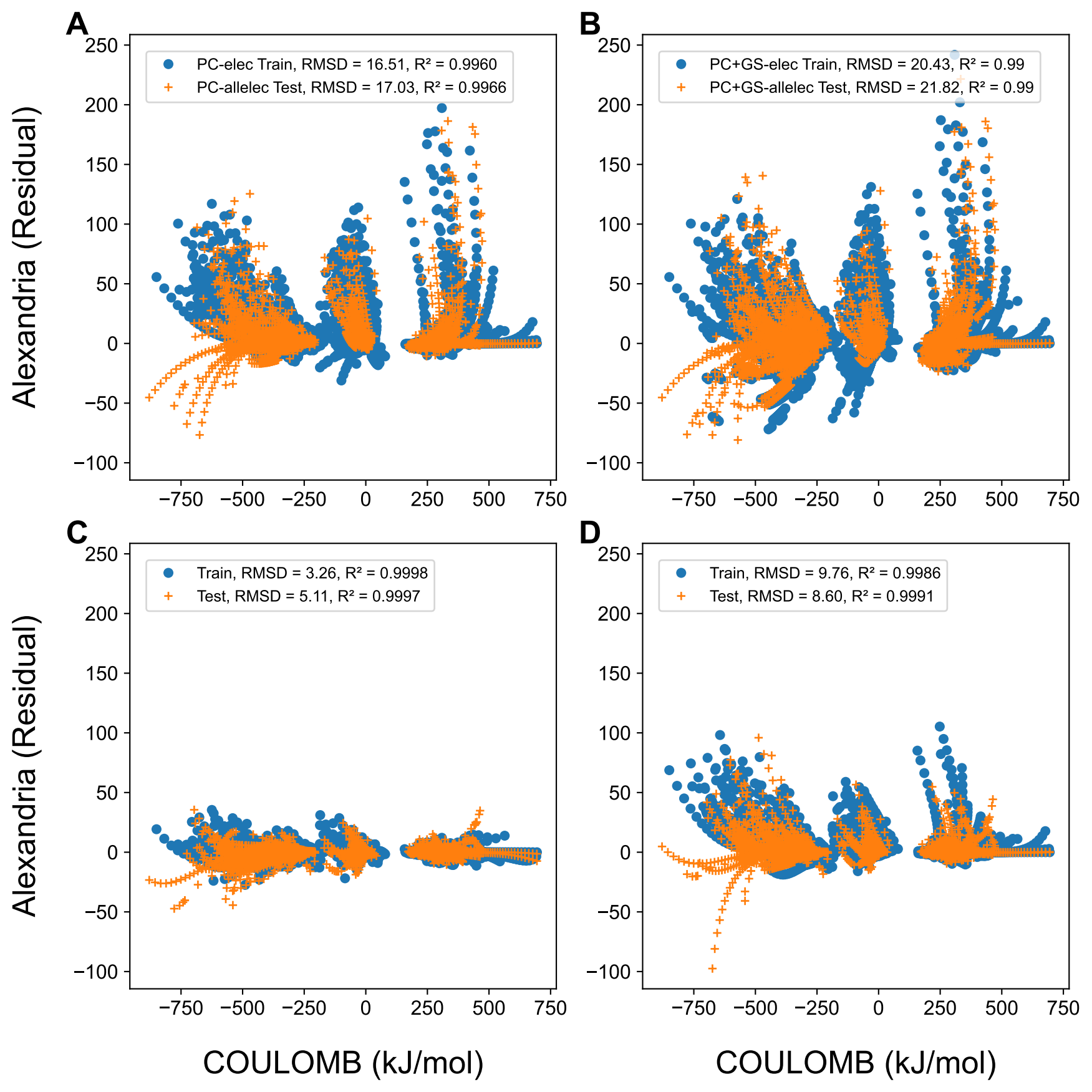
A
PC-elec Train, RMSD = 16.51, R² = 0.9960
PC-allelec Test, RMSD = 17.03, R² = 0.9966
B
PC+GS-elec Train, RMSD = 20.43, R² = 0.99
PC+GS-allelec Test, RMSD = 21.82, R² = 0.99
C
Train, RMSD = 3.26, R² = 0.9998
Test, RMSD = 5.11, R² = 0.9997
D
Train, RMSD = 9.76, R² = 0.9986
Test, RMSD = 8.60, R² = 0.9991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