Li⁺(H₂O)_q decomposition of 2-B energy -20 -40 -60 -(W-W) ion inside E(2-B), kcal/mol -(I-W) ion inside -⊙— (W-W) ion inside (BSSE) -80 -⊡- (I-W) ion inside (BSSE) ─ (W-W) ion outside ■— (I-W) ion outside -100 -⊙— (W-W) ion outside (BSSE) -⊡— (I-W) ion outside (BSSE) -120 -140 -160 aVDZ aVQZ aVTZ aV5Z/V5Z Basis set