## Ionization energies error 0.11 H - 0.00649 0.11 0.59 1.9 0.11 1.4 2.6 He - 2.7 5.4 0.82 0.82 6.1 3.4 4.3 7.1 2.8 12 Li -4.5 0.049 0.12 3.7 1.7 6.2 11 1.4 2.4 7.5 10 12 12 8.8 Be -6.8 6.3 1.5 11 В -8.7 4.7 12 11 8.3 5.7 3.4 4.1 11 10 C -6.5 5.6 9.7 9.5 4.6 3.6 1.8 2.3 13 error [kcal/mol] N -4.5 6 5.8 6.3 0.98 1.6 5.3 1.3 14 10 1.6 3 2.3 9.6 5.5 3.8 5.7 4.4 0 -8 F -5.4 3.7 2.7 4.6 2.3 4.6 9.7 2.1 2.7 System Ne - 2.1 5.4 4 1.9 0.97 0.032 2.5 3.3 13 Na - 5.1 2.1 0.94 0.39 4.9 0.13 3.3 10 Mg - 0.794 6.4 1.3 1.6 3 8.7 5.8 0.097 abs. AI - 2.1 0.28 4.7 4.4 0.98 0.53 3.5 0.71 3.5 1 Si -1 0.34 3.8 3.8 2.8 1.6 4.6 3.6 P - 0.0110.42 3 3.1 4.3 2.3 3.1 0.57 3.5 S - 1.60.51 0.86 0.44 2.2 1.3 0.49 1.5 5.1 2 0.038 CI -0.021 0.31 1.2 8.0 0.27 1.3 3.1 4.8 Ar - 1.4 0.5 0.022 1.7 0.26 0.66 0.45 1.4 3.1 MAE -3.6 3.4 3.9 3.7 3.5 2.3 3.2 2.9 7.4 ı Т PBE **AM05** SCAN **B3LYP B97 M**06 **R2SCAN** M08-HX SOGGA11