## 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 0.097 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 9.8 9.5 4.6 3.6 1.8 2.3 13 error [kcal/mol] N -4.5 6 5.7 6.3 0.98 1.6 5.3 1.3 14 10 1.6 3.3 2.3 9.6 5.5 3.8 5.7 4.4 0 -8 F -5.4 2.9 2.7 4.6 2.3 4.6 9.7 3.7 2.7 System Ne - 2.1 5.4 2.9 1.9 0.95 0.03 2.6 3.3 13 Na -5.1 2.1 0.93 0.38 4.9 0.13 3.3 10 Mg - 0.794 5.9 6.4 1.3 1.6 3 8.7 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 2.9 3.1 4.3 2.3 3.1 0.57 3.5 S - 1.60.51 1.1 0.43 2.2 1.3 0.49 1.5 5.1 2 0.038 CI -0.021 0.31 0.94 0.75 0.27 1.3 3.1 4.8 Ar - 1.4 0.074 1.7 0.26 0.18 0.66 0.43 1.4 3.1 MAE -3.6 3.4 3.9 3.7 3.5 2.3 3.2 2.9 ı Т PBE **AM05** SCAN **B3LYP B97 M**06 **R2SCAN** M08-HX SOGGA11