Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Extending Conceptual DFT to include Additional Variables: Oriented External Electric Field

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Table S1. The dihalogens: sensitivity of I, A, μ and η for a perpendicular field (all values in a.u.).

	∂I/∂ε	∂A/∂ε	∂μ/∂ε	∂η/∂ε
F_2	+0.016	+0.060	+0.038	-0.027
Cl_2	+0.047	+0.146	+0.112	-0.053
Br_2	+0.067	+0.166	+0.120	-0.046
I_2	+0.100	+0.200	+0.150	-0.046

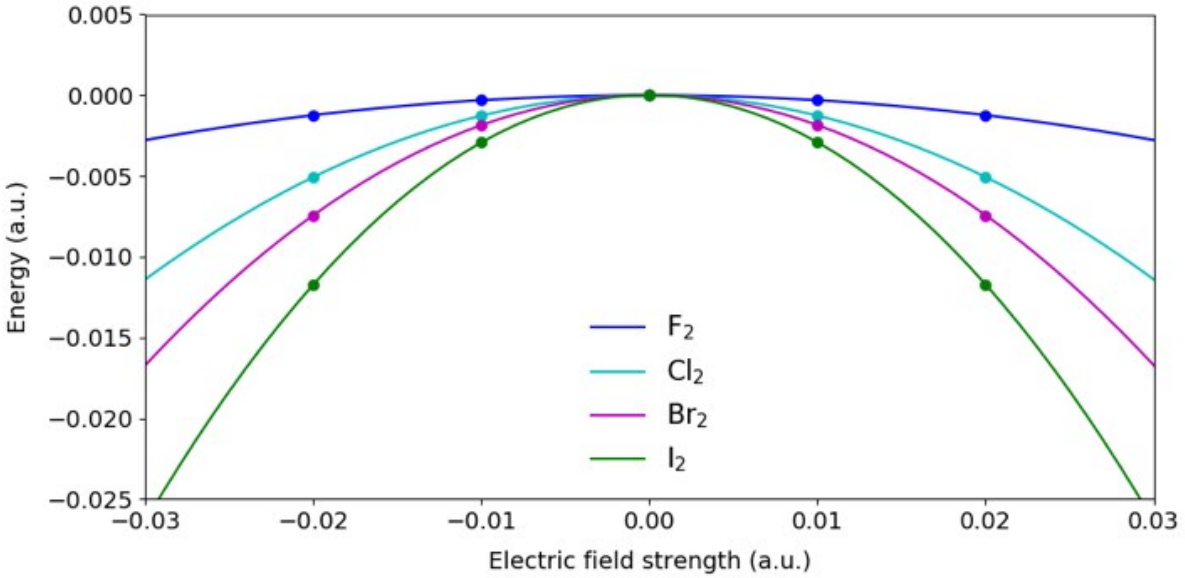

Figure S1. The dihalogens: energy vs electric field strength for a perpendicular field (all values in a.u.).

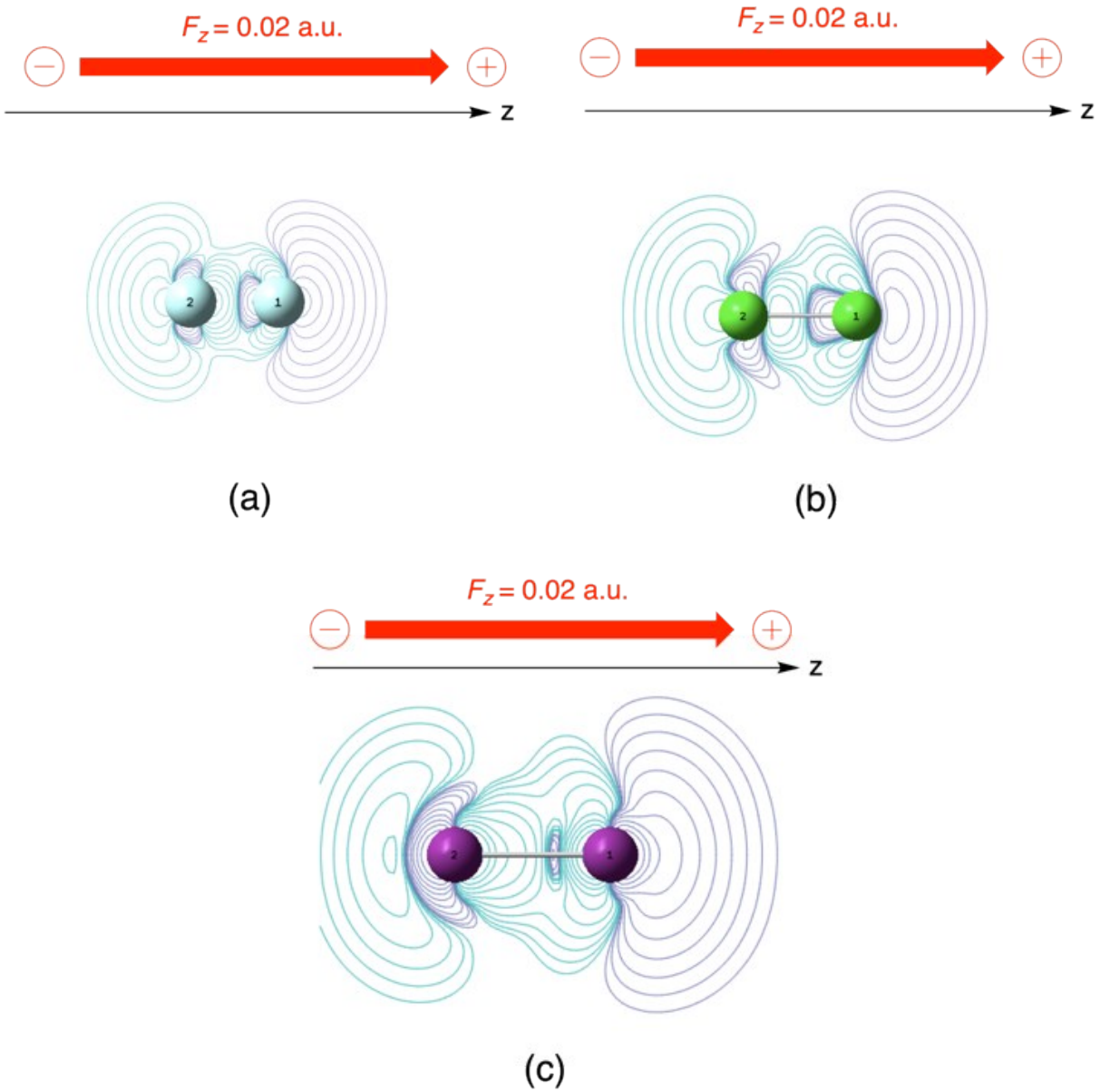

Figure S2. (∂ρ(**r**)/∂ε) (polarization or induced density) plots for F_2, Cl_2 and I_2 for a parallel field F_z of +0.02 a.u. (blue: positive contours; green blue: negative contours).

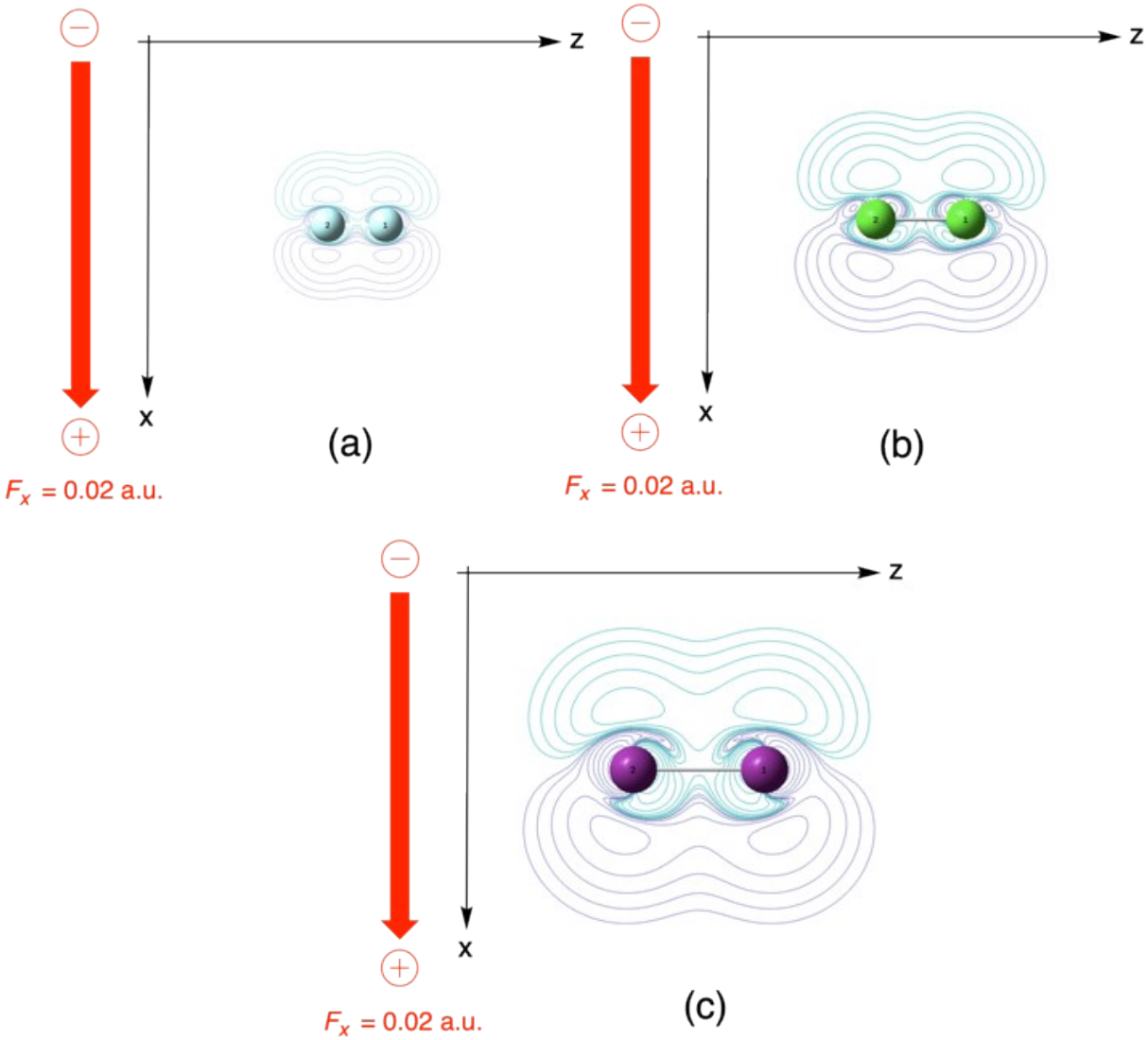

Figure S3. (∂ρ(**r**)/∂ε) (polarization or induced density) plots for F_2, Cl_2 and I_2 for a perpendicular field of F_x of +0.02 a.u. (blue: positive contours ; green blue : negative contours)

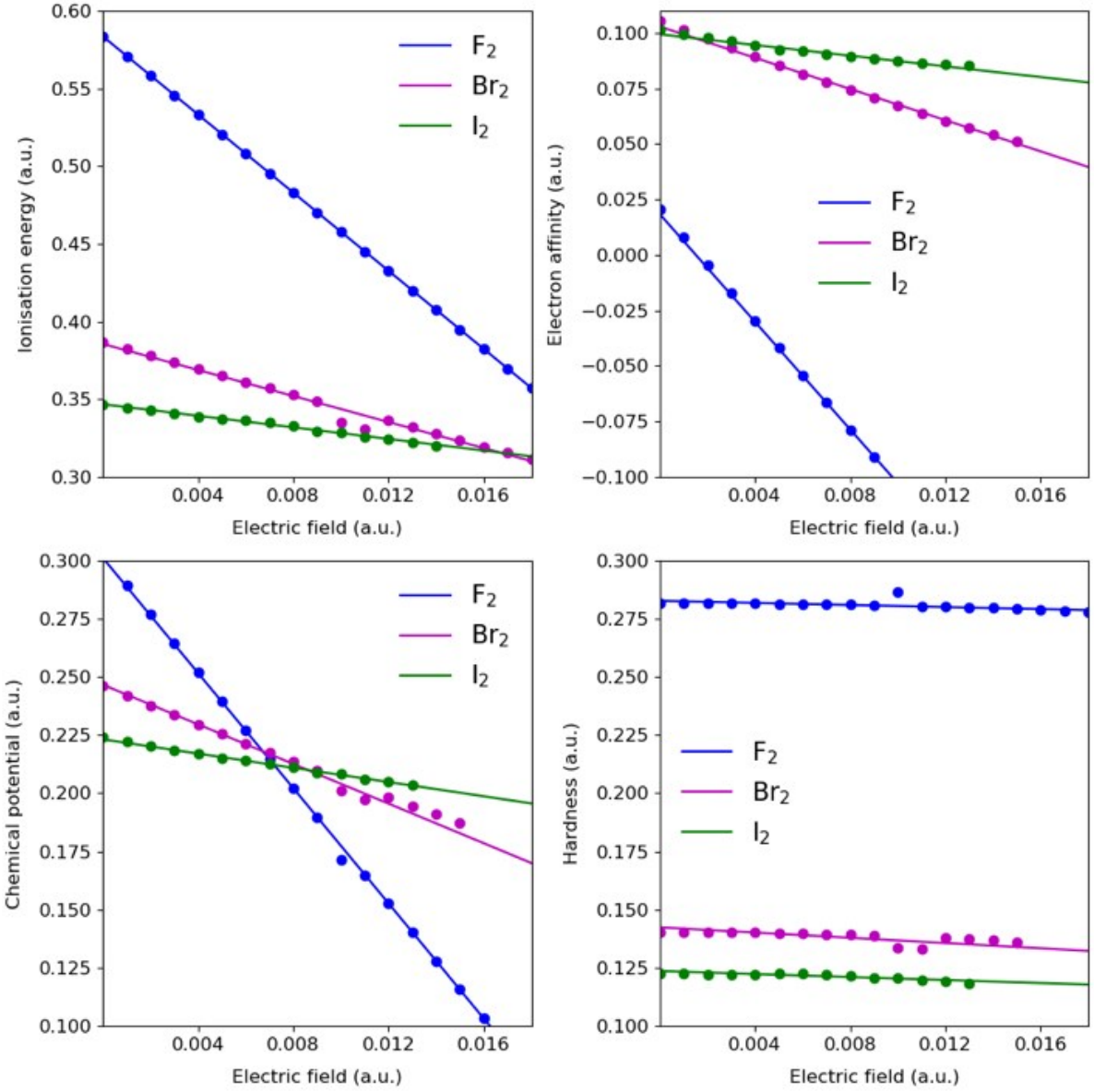

Figure S4. Evolution of I, A, μ and η as a function of ε for a perpendicular field for F_2, Br_2, I_2