**Impact of Non-Empirically Tuning the Range-Separation Parameter of Long-Range Corrected Hybrid Functionals on Ionization Potentials, Electron Affinities, and Fundamental Gaps**

Talapunur Vikramaditya,[[1]](#endnote-1) Jeng-Da Chai,[[2]](#endnote-2)\* and Shiang-Tai Lini\*

1. T. Vikramaditya, Shiang-Tai Lin

   Computational Molecular Engineering Laboratory,Department of Chemical Engineering, National Taiwan University, Taipei 10617, Taiwan. [↑](#endnote-ref-1)
2. Jeng-Da Chai

   Department of Physics, Center for Theoretical Physics, and Center for Quantum Science and Engineering, National Taiwan University, Taipei 10617, Taiwan.

   **Supporting Information**

   Table 1. CCSD(T)//ATZ IP, EA and FG evaluated employing ∆SCF approach

   (30 compounds).

   |  |  |  |  |
   | --- | --- | --- | --- |
   | **Compounds** | **IP** | **EA** | **FG** |
   | Butyl amine | 9.44 | -0.57 | 10.01 |
   | Cyclohexyl amine | 9.3 | -0.53 | 9.83 |
   | Dimethyl amine | 8.94 | -0.61 | 9.55 |
   | Sec-Butyl amine | 9.31 | -0.56 | 9.87 |
   | Butanol | 10.68 | -0.74 | 11.42 |
   | Ethyleneglycol | 10.97 | -0.7 | 11.67 |
   | Phenol | 9.2 | -0.49 | 9.69 |
   | Quinol | 8.99 | -0.59 | 9.58 |
   | 1-Butyne | 10.38 | -0.59 | 10.97 |
   | Butadine | 9.22 | -0.78 | 10 |
   | 1,4-Cyclohexadine | 9.08 | -0.79 | 9.87 |
   | Benzene | 9.43 | -0.79 | 10.22 |
   | Naphthalene | 8.23 | -0.63 | 8.86 |
   | Acridine | 8.06 | 0.54 | 7.52 |
   | Azulene | 7.54 | 0.41 | 7.13 |
   | Furan | 9.05 | -0.83 | 9.88 |
   | Thiophene | 9.39 | -0.77 | 10.16 |
   | Pyridine | 9.73 | -0.74 | 10.47 |
   | Indole | 7.93 | -0.38 | 8.31 |
   | Quinoline | 8.77 | -0.59 | 9.36 |
   | Carbazole | 7.78 | -0.36 | 8.14 |
   | Benzonitrile | 9.89 | -0.32 | 10.21 |
   | meta Cyano Benzonitrile | 10.41 | 0.52 | 9.89 |
   | TCNE | 11.96 | 2.92 | 9.04 |
   | Fumeronitrile | 11.41 | 0.88 | 10.53 |
   | Benzoquinone | 10.17 | 1.47 | 8.7 |
   | F4- Benzoquinone | 11.01 | 2.18 | 8.83 |
   | Benzaldehyde | 9.85 | -0.06 | 9.91 |
   | Maleic Anhydride | 11.21 | 0.94 | 10.27 |
   | Pthalimide | 10.02 | 0.55 | 9.47 |

   **Table 2. LC-ωPBE//ATZ IP, EA and FG evaluated employing ∆SCF approach with default range separation parameter (ω=0.40 bohr-1). (30 compounds).**

   |  |  |  |  |
   | --- | --- | --- | --- |
   | **Compounds** | **IP** | **EA** | **FG** |
   | Butyl amine | 9.37 | -0.58 | 9.95 |
   | Cyclohexyl amine | 9.22 | -0.57 | 9.79 |
   | Dimethyl amine | 8.9 | -0.62 | 9.52 |
   | Sec-Butyl amine | 9.28 | -0.59 | 9.87 |
   | Butanol | 10.59 | -0.56 | 11.15 |
   | Ethyleneglycol | 10.83 | -0.73 | 11.56 |
   | Phenol | 9.16 | -0.53 | 9.69 |
   | Quinol | 8.94 | -0.67 | 9.61 |
   | 1-Butyne | 10.25 | -0.6 | 10.85 |
   | Butadine | 9.1 | -0.79 | 9.89 |
   | 1,4-Cyclohexadine | 9.03 | -0.81 | 9.84 |
   | Benzene | 9.42 | -0.8 | 10.22 |
   | Naphthalene | 8.31 | -0.43 | 8.74 |
   | Acridine | 8.12 | 0.75 | 7.37 |
   | Azulene | 7.35 | 0.78 | 6.57 |
   | Furan | 9.03 | -0.81 | 9.84 |
   | Thiophene | 9.42 | -0.79 | 10.21 |
   | Pyridine | 9.67 | -0.89 | 10.56 |
   | Indole | 8.01 | -0.38 | 8.39 |
   | Quinoline | 8.82 | -0.02 | 8.84 |
   | Carbazole | 7.84 | -0.39 | 8.23 |
   | Benzonitrile | 9.94 | -0.09 | 10.03 |
   | meta Cyano Benzonitrile | 10.49 | 0.78 | 9.71 |
   | TCNE | 12.03 | 3.41 | 8.62 |
   | Fumeronitrile | 11.41 | 1.26 | 10.15 |
   | Benzoquinone | 10.67 | 1.74 | 8.93 |
   | F4- Benzoquinone | 11.06 | 2.48 | 8.58 |
   | Benzaldehyde | 9.8 | 0.15 | 9.65 |
   | Maleic Anhydride | 11.63 | 1.23 | 10.4 |
   | Pthalimide | 10.09 | 0.71 | 9.38 |

   **Table 3. Tuned IP, EA evaluated employing ∆SCF approach using eq. 3 with LC-ωPBE//ATZ (30 compounds).**

   |  |  |  |  |
   | --- | --- | --- | --- |
   | **Compounds** | **ω** | **IP** | **EA** |
   | Butyl amine | 0.35 | 9.36 | -0.57 |
   | Cyclohexyl amine | 0.33 | 9.18 | -0.55 |
   | Dimethyl amine | 0.35 | 8.89 | -0.62 |
   | Sec-Butyl amine | 0.34 | 9.26 | -0.58 |
   | Butanol | 0.38 | 10.56 | -0.56 |
   | Ethyleneglycol | 0.4 | 10.83 | -0.73 |
   | Phenol | 0.28 | 9.11 | -0.5 |
   | Quinol | 0.28 | 8.87 | -0.63 |
   | 1-Butyne | 0.34 | 10.22 | -0.59 |
   | Butadine | 0.31 | 9.06 | -0.78 |
   | 1,4-Cyclohexadiene | 0.3 | 8.82 | -0.8 |
   | Benzene | 0.28 | 9.38 | -0.78 |
   | Naphthalene | 0.26 | 8.17 | -0.35 |
   | Acridine | 0.24 | 7.89 | 0.82 |
   | Azulene | 0.24 | 7.37 | 0.68 |
   | Furan | 0.31 | 9.01 | -0.8 |
   | Thiophene | 0.36 | 9.42 | -0.79 |
   | Pyridine | 0.31 | 9.6 | -0.88 |
   | Indole | 0.27 | 7.9 | -0.35 |
   | Quinoline | 0.26 | 8.68 | 0.05 |
   | Carbazole | 0.24 | 7.66 | -0.48 |
   | Benzonitrile | 0.28 | 9.82 | -0.06 |
   | meta Cyano Benzonitrile | 0.27 | 10.3 | 0.8 |
   | TCNE | 0.3 | 11.76 | 3.36 |
   | Fumeronitrile | 0.33 | 11.3 | 1.26 |
   | Benzoquinone | 0.39 | 10.63 | 1.75 |
   | F4- Benzoquinone | 0.3 | 10.8 | 2.49 |
   | Benzaldehyde | 0.31 | 9.7 | 0.19 |
   | Maleic Anhydride | 0.43 | 11.72 | 1.22 |
   | Pthalimide | 0.3 | 10 | 0.76 |

   **Table 4. Tuned EA, evaluated employing ∆SCF approach using eq. 4 with LC-ωPBE//ATZ (26 compounds).**

   |  |  |  |
   | --- | --- | --- |
   | **Compounds** | **ω** | **EA** |
   | Butyl amine | 0.11 | -0.42 |
   | Cyclohexyl amine | 0.11 | -0.39 |
   | Dimethyl amine | 0.11 | -0.45 |
   | Sec-Butyl amine | 0.12 | -0.43 |
   | Butanol | 0.11 | -0.40 |
   | Ethyleneglycol | 0.39 | -0.73 |
   | Phenol | 0.13 | -0.39 |
   | Quinol | 0.18 | -0.54 |
   | 1-Butyne | 0.11 | -0.43 |
   | Butadine | 0.27 | -0.77 |
   | Naphthalene | 0.24 | -0.33 |
   | Acridine | 0.23 | 0.82 |
   | Azulene | 0.23 | 0.67 |
   | Thiophene | 0.36 | -0.79 |
   | Indole | 0.21 | -0.32 |
   | Quinoline | 0.25 | 0.05 |
   | Carbazole | 0.23 | -0.47 |
   | Benzonitrile | 0.26 | -0.05 |
   | meta Cyano Benzonitrile | 0.25 | 0.81 |
   | TCNE | 0.27 | 3.35 |
   | Fumeronitrile | 0.3 | 1.27 |
   | Benzoquinone | 0.29 | 1.81 |
   | F4- Benzoquinone | 0.3 | 2.49 |
   | Benzaldehyde | 0.27 | 0.21 |
   | Maleic Anhydride | 0.31 | 1.26 |
   | Pthalimide | 0.26 | 0.78 |

   **Table 5. Tuned IP, EA, FG employing ∆SCF approach using eq. 5 with LC-ωPBE//ATZ (30 compounds).**

   |  |  |  |  |  |
   | --- | --- | --- | --- | --- |
   | **Compounds** | **ω** | **IP** | **EA** | **FG** |
   | Butyl amine | 0.35 | 9.36 | -0.57 | 9.93 |
   | Cyclohexyl amine | 0.33 | 9.18 | -0.55 | 9.73 |
   | Dimethyl amine | 0.35 | 8.89 | -0.62 | 9.51 |
   | Sec-Butyl amine | 0.34 | 9.26 | -0.58 | 9.84 |
   | Butanol | 0.38 | 10.56 | -0.56 | 11.12 |
   | Ethyleneglycol | 0.4 | 10.83 | -0.73 | 11.56 |
   | Phenol | 0.28 | 9.11 | -0.5 | 9.61 |
   | Quinol | 0.28 | 8.87 | -0.63 | 9.5 |
   | 1-Butyne | 0.34 | 10.22 | -0.59 | 10.81 |
   | Butadine | 0.31 | 9.06 | -0.78 | 9.84 |
   | 1,4-Cyclohexadiene | 0.3 | 8.82 | -0.8 | 9.62 |
   | Benzene | 0.28 | 9.38 | -0.78 | 10.16 |
   | Naphthalene | 0.25 | 8.15 | -0.34 | 8.49 |
   | Acridine | 0.23 | 7.87 | 0.82 | 7.05 |
   | Azulene | 0.23 | 7.38 | 0.67 | 6.71 |
   | Furan | 0.31 | 9.01 | -0.8 | 9.81 |
   | Thiophene | 0.36 | 9.42 | -0.79 | 10.21 |
   | Pyridine | 0.31 | 9.6 | -0.88 | 10.48 |
   | Indole | 0.27 | 7.9 | -0.35 | 8.25 |
   | Quinoline | 0.26 | 8.68 | 0.05 | 8.63 |
   | Carbazole | 0.23 | 7.65 | -0.47 | 8.12 |
   | Benzonitrile | 0.28 | 9.82 | -0.06 | 9.88 |
   | meta Cyano Benzonitrile | 0.27 | 10.3 | 0.8 | 9.5 |
   | TCNE | 0.27 | 11.67 | 3.35 | 8.32 |
   | Fumeronitrile | 0.33 | 11.3 | 1.26 | 10.04 |
   | Benzoquinone | 0.39 | 10.63 | 1.75 | 8.88 |
   | F4- Benzoquinone | 0.3 | 10.8 | 2.49 | 8.31 |
   | Benzaldehyde | 0.3 | 9.69 | 0.19 | 9.5 |
   | Maleic Anhydride | 0.43 | 11.72 | 1.22 | 10.5 |
   | Pthalimide | 0.3 | 10 | 0.76 | 9.24 |

   **Table 6. LC-ωPBE//ADZ IP, EA and FG evaluated employing ∆SCF approach with default range separation parameter (ω=0.40 bohr-1). (30 compounds).**

   |  |  |  |  |
   | --- | --- | --- | --- |
   | **Compounds** | **IP** | **EA** | **FG** |
   | Butyl amine | 9.38 | -0.73 | 10.11 |
   | Cyclohexyl amine | 9.22 | -0.71 | 9.93 |
   | Dimethyl amine | 8.9 | -0.77 | 9.67 |
   | Sec-Butyl amine | 9.29 | -0.74 | 10.03 |
   | Butanol | 10.57 | -0.71 | 11.28 |
   | Ethyleneglycol | 10.8 | -0.88 | 11.68 |
   | Phenol | 9.13 | -0.67 | 9.8 |
   | Quinol | 8.92 | -0.82 | 9.74 |
   | 1-Butyne | 10.19 | -0.74 | 10.93 |
   | Butadine | 9.04 | -1 | 10.04 |
   | 1,4-Cyclohexadine | 8.99 | -1.03 | 10.02 |
   | Benzene | 9.37 | -0.79 | 10.16 |
   | Naphthalene | 8.27 | -0.4 | 8.67 |
   | Acridine | 8.08 | 0.77 | 7.31 |
   | Azulene | 7.32 | 0.8 | 6.52 |
   | Furan | 8.99 | -1 | 9.99 |
   | Thiophene | 9.42 | -1.32 | 10.74 |
   | Pyridine | 9.68 | -0.88 | 10.56 |
   | Indole | 7.97 | -0.49 | 8.46 |
   | Quinoline | 8.77 | 0 | 8.77 |
   | Carbazole | 7.81 | -0.48 | 8.29 |
   | Benzonitrile | 9.89 | -0.07 | 9.96 |
   | meta Cyano Benzonitrile | 10.44 | 0.8 | 9.64 |
   | TCNE | 11.96 | 3.42 | 8.54 |
   | Fumeronitrile | 11.34 | 1.28 | 10.06 |
   | Benzoquinone | 10.67 | 1.77 | 8.9 |
   | F4- Benzoquinone | 11.07 | 2.54 | 8.53 |
   | Benzaldehyde | 9.79 | 0.18 | 9.61 |
   | Maleic Anhydride | 11.61 | 1.27 | 10.34 |
   | Pthalimide | 10.05 | 0.75 | 9.3 |

   **Table 7. Tuned IP, EA, FG employing ∆SCF approach using eq. 5 with LC-ωPBE//ADZ (30 compounds).**

   |  |  |  |  |  |
   | --- | --- | --- | --- | --- |
   | **Compounds** | **ω** | **IP** | **EA** | **FG** |
   | Butyl amine | 0.35 | 9.36 | -0.72 | 10.08 |
   | Cyclohexyl amine | 0.33 | 9.18 | -0.69 | 9.87 |
   | Dimethyl amine | 0.35 | 8.88 | -0.76 | 9.64 |
   | Sec-Butyl amine | 0.34 | 9.26 | -0.72 | 9.98 |
   | Butanol | 0.39 | 10.57 | -0.71 | 11.28 |
   | Ethyleneglycol | 0.4 | 10.8 | -0.88 | 11.68 |
   | Phenol | 0.28 | 9.08 | -0.62 | 9.7 |
   | Quinol | 0.28 | 8.85 | -0.77 | 9.62 |
   | 1-Butyne | 0.34 | 10.16 | -0.73 | 10.89 |
   | Butadine | 0.3 | 9 | -0.86 | 9.86 |
   | 1,4-Cyclohexadine | 0.3 | 8.78 | -1.01 | 9.79 |
   | Benzene | 0.27 | 9.34 | -0.96 | 10.3 |
   | Naphthalene | 0.27 | 8.1 | -0.59 | 8.69 |
   | Acridine | 0.23 | 7.83 | 0.84 | 6.99 |
   | Azulene | 0.23 | 7.34 | 0.69 | 6.65 |
   | Furan | 0.31 | 8.97 | -0.99 | 9.96 |
   | Thiophene | 0.37 | 9.41 | -1.32 | 10.73 |
   | Pyridine | 0.31 | 9.61 | -0.87 | 10.48 |
   | Indole | 0.27 | 7.86 | -0.45 | 8.31 |
   | Quinoline | 0.26 | 8.64 | 0.06 | 8.58 |
   | Carbazole | 0.23 | 7.62 | -0.46 | 8.08 |
   | Benzonitrile | 0.28 | 9.78 | -0.04 | 9.82 |
   | meta Cyano Benzonitrile | 0.27 | 10.25 | 0.81 | 9.44 |
   | TCNE | 0.3 | 11.69 | 3.37 | 8.32 |
   | Fumeronitrile | 0.33 | 11.23 | 1.28 | 9.95 |
   | Benzoquinone | 0.39 | 10.64 | 1.78 | 8.86 |
   | F4- Benzoquinone | 0.3 | 10.82 | 2.55 | 8.27 |
   | Benzaldehyde | 0.3 | 9.67 | 0.21 | 9.46 |
   | Maleic Anhydride | 0.43 | 11.7 | 1.26 | 10.44 |
   | Pthalimide | 0.29 | 9.95 | 0.8 | 9.15 |

   **Table 8. HOMO, LUMO Energies and their gaps using default range separation parameter (0.40 bohr-1) employing LC-ωPBE//ATZ. (30 compounds).**

   |  |  |  |  |
   | --- | --- | --- | --- |
   | **Compounds** | **-HOMO** | **-LUMO** | **Gap(L-H)** |
   | Butyl amine | 9.62 | -0.76 | 10.38 |
   | Cyclohexyl amine | 9.61 | -0.75 | 10.36 |
   | Dimethyl amine | 9.14 | -0.77 | 9.91 |
   | Sec-Butyl amine | 9.63 | -0.76 | 10.39 |
   | Butanol | 10.67 | -0.74 | 11.41 |
   | Ethyleneglycol | 10.82 | -0.76 | 11.58 |
   | Phenol | 9.6 | -0.72 | 10.32 |
   | Quinol | 9.37 | -0.7 | 10.07 |
   | 1-Butyne | 10.52 | -0.77 | 11.29 |
   | Butadine | 9.47 | -0.83 | 10.3 |
   | 1,4-Cyclohexadine | 9.3 | -0.78 | 10.08 |
   | Benzene | 9.86 | -0.77 | 10.63 |
   | Naphthalene | 8.71 | -0.76 | 9.47 |
   | Acridine | 8.52 | 0.31 | 8.21 |
   | Azulene | 7.91 | 0.28 | 7.63 |
   | Furan | 9.38 | -0.78 | 10.16 |
   | Thiophene | 9.57 | -0.78 | 10.35 |
   | Pyridine | 10.21 | -0.67 | 10.88 |
   | Indole | 8.41 | -0.62 | 9.03 |
   | Quinoline | 9.26 | -0.41 | 9.67 |
   | Carbazole | 8.31 | -0.65 | 8.96 |
   | Benzonitrile | 10.36 | -0.46 | 10.82 |
   | meta Cyano Benzonitrile | 10.92 | 0.35 | 10.57 |
   | TCNE | 12.33 | 2.99 | 9.34 |
   | Fumeronitrile | 11.65 | 0.93 | 10.72 |
   | Benzoquinone | 10.69 | 1.43 | 9.26 |
   | F4- Benzoquinone | 11.35 | 2.18 | 9.17 |
   | Benzaldehyde | 10.25 | -0.23 | 10.48 |
   | Maleic Anhydride | 11.55 | 0.94 | 10.61 |
   | Pthalimide | 10.65 | 0.32 | 10.33 |

   **Table 9. HOMO, LUMO Energies and their gaps tuned using eq. 5 employing LC-ωPBE//ATZ. (30 compounds).**

   |  |  |  |  |
   | --- | --- | --- | --- |
   | **Compounds** | **-HOMO** | **-LUMO** | **GAP(L-H)** |
   | Butyl amine | 9.33 | -0.75 | 10.08 |
   | Cyclohexyl amine | 9.18 | -0.73 | 9.91 |
   | Dimethyl amine | 8.86 | -0.76 | 9.62 |
   | Sec-Butyl amine | 9.28 | -0.75 | 10.03 |
   | Butanol | 10.54 | -0.74 | 11.28 |
   | Ethyleneglycol | 10.82 | -0.76 | 11.58 |
   | Phenol | 9.11 | -0.68 | 9.79 |
   | Quinol | 8.88 | -0.66 | 9.54 |
   | 1-Butyne | 10.21 | -0.76 | 10.97 |
   | Butadine | 9.08 | -0.81 | 9.89 |
   | 1,4-Cyclohexadine | 8.82 | -0.75 | 9.57 |
   | Benzene | 9.37 | -0.74 | 10.11 |
   | Naphthalene | 8.12 | -0.36 | 8.48 |
   | Acridine | 7.84 | 0.79 | 7.05 |
   | Azulene | 7.33 | 0.68 | 6.65 |
   | Furan | 9 | -0.76 | 9.76 |
   | Thiophene | 9.42 | -0.78 | 10.2 |
   | Pyridine | 9.62 | -0.65 | 10.27 |
   | Indole | 7.89 | -0.58 | 8.47 |
   | Quinoline | 8.69 | 0 | 8.69 |
   | Carbazole | 7.61 | -0.49 | 8.1 |
   | Benzonitrile | 9.83 | -0.12 | 9.95 |
   | meta Cyano Benzonitrile | 10.3 | 0.72 | 9.58 |
   | TCNE | 11.56 | 3.35 | 8.21 |
   | Fumeronitrile | 11.29 | 1.15 | 10.14 |
   | Benzoquinone | 10.63 | 1.45 | 9.18 |
   | F4- Benzoquinone | 10.78 | 2.49 | 8.29 |
   | Benzaldehyde | 9.65 | 0.08 | 9.57 |
   | Maleic Anhydride | 11.73 | 0.86 | 10.87 |
   | Pthalimide | 10.02 | 0.61 | 9.41 |

   |  |  |  |  |  |  |
   | --- | --- | --- | --- | --- | --- |
   |  |  |  |  |  |  |
   | **Compounds** | **ω=0.20** | **ω=0.30** | **ω=0.40** | **ω=0.50** | **ω=0.60** |
   | Butyl amine | -0.65 | -0.73 | -0.76 | -0.77 | -0.77 |
   | Cyclohexyl amine | -0.64 | -0.72 | -0.75 | -0.76 | -0.77 |
   | Dimethyl amine | -0.67 | -0.75 | -0.77 | -0.79 | -0.79 |
   | Sec-Butyl amine | -0.64 | -0.73 | -0.76 | -0.77 | -0.78 |
   | Butanol | -0.63 | -0.71 | -0.74 | -0.76 | -0.76 |
   | Ethyleneglycol | -0.64 | -0.73 | -0.76 | -0.78 | -0.78 |
   | Phenol | -0.6 | -0.69 | -0.72 | -0.73 | -0.74 |
   | Quinol | -0.58 | -0.67 | -0.7 | -0.71 | -0.72 |
   | 1-Butyne | -0.66 | -0.74 | -0.77 | -0.78 | -0.79 |
   | Butadine | -0.39 | -0.81 | -0.83 | -0.83 | -0.84 |
   | 1,4-Cyclohexadine | -0.66 | -0.75 | -0.78 | -0.79 | -0.79 |
   | Benzene | -0.67 | -0.75 | -0.77 | -0.78 | -0.79 |
   | Naphthalene | -0.1 | -0.55 | -0.76 | -0.77 | -0.77 |
   | Acridine | 0.93 | 0.53 | 0.31 | 0.17 | 0.08 |
   | Azulene | 0.81 | 0.46 | 0.28 | 0.18 | 0.1 |
   | Furan | -0.7 | -0.76 | -0.78 | -0.79 | -0.79 |
   | Thiophene | -0.7 | -0.76 | -0.78 | -0.79 | -0.79 |
   | Pyridine | -0.44 | -0.65 | -0.67 | -0.68 | -0.68 |
   | Indole | -0.52 | -0.59 | -0.62 | -0.63 | -0.64 |
   | Quinoline | 0.31 | -0.15 | -0.41 | -0.57 | -0.68 |
   | Carbazole | -0.33 | -0.62 | -0.65 | -0.66 | -0.66 |
   | Benzonitrile | 0.29 | -0.2 | -0.46 | -0.55 | -0.55 |
   | meta Cyano Benzonitrile | 1.08 | 0.61 | 0.35 | 0.21 | 0.11 |
   | TCNE | 3.24 | 3.24 | 2.99 | 3.24 | 3.24 |
   | Fumeronitrile | 1.84 | 1.27 | 0.93 | 0.73 | 0.6 |
   | Benzoquinone | 2.36 | 1.78 | 1.43 | 1.21 | 1.08 |
   | F4- Benzoquinone | 3.01 | 2.49 | 2.18 | 1.99 | 1.87 |
   | Benzaldehyde | 0.62 | 0.08 | -0.23 | -0.42 | -0.54 |
   | Maleic Anhydride | 1.92 | 1.31 | 0.94 | 0.72 | 0.58 |
   | Pthalimide | 1.12 | 0.61 | 0.32 | 0.14 | 0.03 |

   **Table 10. Negative LUMO energies at various range separation parameters (0.20, 0.30, 0.40, 0.50, 0.60 bohr-1) with LC-ωPBE//ATZ. (30 compounds).**

   **Table 11. Default and tuned (ω) based on eq. 5 IP, EA and FG (∆SCF) of LC-BLYP//ATZ. (30 compounds).**

   |  |  |  |  |  |  |  |  |
   | --- | --- | --- | --- | --- | --- | --- | --- |
   |  | **Default ω** | | |  | **Tuned ω** | | |
   |  | **IP** | **EA** | **FG** |  | **IP** | **EA** | **FG** |
   | Butyl amine | 9.4 | -0.66 | 10.06 |  | 9.37 | -0.64 | 10.01 |
   | Cyclohexyl amine | 9.25 | -0.65 | 9.9 |  | 9.19 | -0.61 | 9.8 |
   | Dimethyl amine | 9.73 | -0.61 | 10.34 |  | 9.6 | -0.59 | 10.19 |
   | Sec-Butyl amine | 9.33 | -0.66 | 9.99 |  | 9.29 | -0.63 | 9.92 |
   | Butanol | 10.71 | -0.64 | 11.35 |  | 10.59 | -0.62 | 11.21 |
   | Ethyleneglycol | 11.22 | -0.68 | 11.9 |  | 11.22 | -0.68 | 11.9 |
   | Phenol | 9.19 | -0.61 | 9.8 |  | 9.14 | -0.55 | 9.69 |
   | Quinol | 8.97 | -0.53 | 9.5 |  | 8.91 | -0.66 | 9.57 |
   | 1-Butyne | 10.33 | -0.68 | 11.01 |  | 10.29 | -0.65 | 10.94 |
   | Butadine | 9.15 | -0.76 | 9.91 |  | 9.15 | -0.95 | 10.1 |
   | 1,4-Cyclohexadine | 9.09 | -0.69 | 9.78 |  | 8.87 | -0.65 | 9.52 |
   | Benzene | 9.45 | -0.69 | 10.14 |  | 9.45 | -0.88 | 10.33 |
   | Naphthalene | 8.34 | -0.68 | 9.02 |  | 8.15 | -0.37 | 8.52 |
   | Acridine | 8.15 | 0.66 | 7.49 |  | 7.83 | 0.78 | 7.05 |
   | Azulene | 7.35 | 0.72 | 6.63 |  | 7.38 | 0.63 | 6.75 |
   | Furan | 9.1 | -0.7 | 9.8 |  | 9.09 | -0.68 | 9.77 |
   | Thiophene | 9.42 | -0.7 | 10.12 |  | 9.43 | -0.69 | 10.12 |
   | Pyridine | 9.73 | -0.57 | 10.3 |  | 9.68 | -0.9 | 10.58 |
   | Indole | 8.04 | -0.48 | 8.52 |  | 7.9 | -0.42 | 8.32 |
   | Quinoline | 8.85 | -0.1 | 8.95 |  | 8.68 | 0.02 | 8.66 |
   | Carbazole | 7.87 | -0.49 | 8.36 |  | 7.67 | -0.51 | 8.18 |
   | Benzonitrile | 9.99 | -0.43 | 10.42 |  | 9.83 | -0.09 | 9.92 |
   | meta Cyano Benzonitrile | 10.56 | 0.72 | 9.84 |  | 10.3 | 0.76 | 9.54 |
   | TCNE | 12.19 | 3.39 | 8.8 |  | 11.73 | 3.32 | 8.41 |
   | Fumeronitrile | 11.52 | 1.21 | 10.31 |  | 11.32 | 1.24 | 10.08 |
   | Benzoquinone | 10.94 | 1.7 | 9.24 |  | 10.5 | 1.79 | 8.71 |
   | F4- Benzoquinone | 11.28 | 2.51 | 8.77 |  | 10.89 | 2.53 | 8.36 |
   | Benzaldehyde | 9.91 | 0.1 | 9.81 |  | 9.72 | 0.19 | 9.53 |
   | Maleic Anhydride | 11.89 | 1.21 | 10.68 |  | 11.59 | 1.26 | 10.33 |
   | Pthalimide | 10.17 | 0.68 | 9.49 |  | 10 | 0.77 | 9.23 |

   **Table 12.** **Default and tuned (ω) based on eq. 5 IP, EA and FG (∆SCF) of ωB97XD//ATZ. (30 compounds).**

   |  |  |  |  |  |  |  |  |
   | --- | --- | --- | --- | --- | --- | --- | --- |
   |  | **Default ω** | | |  | **Tuned ω** | | |
   |  | **IP** | **EA** | **FG** |  | **IP** | **EA** | **FG** |
   | Butyl amine | 9.29 | -0.64 | 9.93 |  | 9.41 | -0.64 | 10.05 |
   | Cyclohexyl amine | 9.12 | -0.63 | 9.75 |  | 9.22 | -0.63 | 9.85 |
   | Dimethyl amine | 8.82 | -0.69 | 9.51 |  | 9.72 | -0.6 | 10.32 |
   | Sec-Butyl amine | 9.17 | -0.65 | 9.82 |  | 9.27 | -0.65 | 9.92 |
   | Butanol | 10.51 | -0.63 | 11.14 |  | 10.64 | -0.62 | 11.26 |
   | Ethyleneglycol | 10.57 | -0.69 | 11.26 |  | 11.28 | -0.69 | 11.97 |
   | Phenol | 9.01 | -0.59 | 9.6 |  | 9.06 | -0.59 | 9.65 |
   | Quinol | 8.78 | -0.7 | 9.48 |  | 8.83 | -0.63 | 9.46 |
   | 1-Butyne | 10.11 | -0.65 | 10.76 |  | 10.25 | -0.65 | 10.9 |
   | Butadine | 8.92 | -0.99 | 9.91 |  | 9.02 | -0.98 | 10 |
   | 1,4-Cyclohexadine | 8.72 | -0.71 | 9.43 |  | 8.88 | -0.7 | 9.58 |
   | Benzene | 9.28 | -0.83 | 10.11 |  | 9.34 | -0.69 | 10.03 |
   | Naphthalene | 8.06 | -0.5 | 8.56 |  | 8.08 | -0.49 | 8.57 |
   | Acridine | 7.81 | 0.67 | 7.14 |  | 7.79 | 0.66 | 7.13 |
   | Azulene | 7.28 | 0.54 | 6.74 |  | 7.27 | 0.52 | 6.75 |
   | Furan | 8.88 | -0.68 | 9.56 |  | 8.98 | -0.68 | 9.66 |
   | Thiophene | 9.34 | -0.68 | 10.02 |  | 9.45 | -0.67 | 10.12 |
   | Pyridine | 9.56 | -1.01 | 10.57 |  | 9.62 | -0.54 | 10.16 |
   | Indole | 7.8 | -0.44 | 8.24 |  | 7.86 | -0.44 | 8.3 |
   | Quinoline | 9.27 | -0.1 | 9.37 |  | 9.5 | -0.53 | 10.03 |
   | Carbazole | 7.61 | -0.63 | 8.24 |  | 7.59 | -0.64 | 8.23 |
   | Benzonitrile | 9.72 | -0.2 | 9.92 |  | 9.78 | -0.18 | 9.96 |
   | meta Cyano Benzonitrile | 10.22 | 0.67 | 9.55 |  | 10.27 | 0.68 | 9.59 |
   | TCNE | 11.61 | 3.25 | 8.36 |  | 11.76 | 3.3 | 8.46 |
   | Fumeronitrile | 11.1 | 1.15 | 9.95 |  | 11.31 | 1.19 | 10.12 |
   | Benzoquinone | 10.24 | 1.69 | 8.55 |  | 10.72 | 1.71 | 9.01 |
   | F4- Benzoquinone | 10.7 | 2.35 | 8.35 |  | 10.87 | 2.39 | 8.48 |
   | Benzaldehyde | 9.87 | 0.06 | 9.81 |  | 9.68 | 0.08 | 9.6 |
   | Maleic Anhydride | 11.2 | 1.11 | 10.09 |  | 11.72 | 1.17 | 10.55 |
   | Pthalimide | 10.1 | 0.63 | 9.47 |  | 10.15 | 0.64 | 9.51 |

   [↑](#endnote-ref-2)