**Supporting information**

MS Title: Structured Water Chains in External Electric Fields  
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Table caption: HOMO-LUMO gap as a function of electric field strength for 5-units of pentamer chain. The structure could not be optimized at smaller field strengths with the ωB97X-D and M06-2X functionals.

Table I: HOMO-LUMO gap as a function of electric field strength for 5-units of pentamer chain. The structure could not be optimized at smaller field strengths with the ωB97X-D and M06-2X functionals.

|  |  |  |  |
| --- | --- | --- | --- |
| Field  (a.u.) | B3LYP  (eV) | ωB97X-D  (eV) | M06-2X  (eV) |
| 0.005 | 3.77 | -- | -- |
| 0.010 | 4.24 | 8.35 | -- |
| 0.020 | 5.09 | 9.20 | 7.95 |
| 0.030 | 5.93 | 10.0 | 8.79 |
| 0.040 | 6.69 | 10.6 | 9.15 |
| 0.050 | 6.90 | 10.8 | 9.31 |
| 0.060 | 6.52 | 10.4 | 9.61 |
| 0.070 | 5.96 | 9.88 | 8.28 |
| 0.080 | 5.36 | 9.27 | 7.65 |
| 0.090 | 4.70 | 8.61 | 6.98 |
| 0.100 | 4.02 | 7.90 | 6.27 |
| 0.110 | 3.30 | 7.16 | 5.53 |
| 0.120 | 2.56 | 6.39 | 4.77 |
| 0.130 | 1.79 | 5.59 | 3.99 |
| 0.140 | 1.00 | 4.77 | 3.21 |
| 0.150 | 0.22 | 3.95 | 2.44 |