

Comparison of Calculated and Experimental HOMO-LUMO Gaps for C28 with Varying Parameters

| hopping | U | K | hf H-L gap | TB H-L gap | Exp H-L gap:3.38 | Excitation energy |
|---------|------|-----|------------|------------|------------------|-------------------|
| -2.4 | -1.0 | 5.0 | 2.332 | 2.249 | 3.38 | 2.352039e+00 [eV] |
| -3.0 | -1.0 | 5.0 | 2.894 | 2.811 | 3.38 | 2.899927e+00 [eV] |
| -3.1 | -1.0 | 5.0 | 2.988 | 2.904 | 3.38 | 2.991886e+00 [eV] |
| -3.2 | -1.0 | 5.0 | 3.082 | 2.998 | 3.38 | 3.083975e+00 [eV] |
| -3.3 | -1.0 | 5.0 | 3.175 | 3.092 | 3.38 | 3.176177e+00 [eV] |
| -3.4 | -1.0 | 5.0 | 3.269 | 3.186 | 3.38 | 3.268480e+00 [eV] |
| -3.5 | -1.0 | 5.0 | 3.363 | 3.279 | 3.38 | 3.360874e+00 [eV] |
| -3.6 | -1.0 | 5.0 | 3.456 | 3.373 | 3.38 | 3.453350e+00 [eV] |
| -3.7 | -1.0 | 5.0 | 3.550 | 3.467 | 3.38 | 3.545894e+00 [eV] |
| -3.8 | -1.0 | 5.0 | 3.644 | 3.560 | 3.38 | 3.638519e+00 [eV] |
| -3.9 | -1.0 | 5.0 | 3.738 | 3.659 | 3.38 | 3.731200e+00 [eV] |
| -4.0 | -1.0 | 5.0 | 3.831 | 3.748 | 3.38 | 3.823937e+00 [eV] |

Table 1

| U | hopping | K | hf H-L gap | TB H-L gap | Exp H-L gap:3.38 | Excitation energy |
|--------|---------|-----|------------|------------|------------------|-------------------|
| -0.001 | -4.0 | 5.0 | 3.748 | 3.748 | 3.38 | 3.747741e+00 [eV] |
| -0.01 | -4.0 | 5.0 | 3.749 | 3.748 | 3.38 | 3.748128e+00 [eV] |
| -0.1 | -4.0 | 5.0 | 3.756 | 3.748 | 3.38 | 3.752264e+00 [eV] |
| -0.3 | -4.0 | 5.0 | 3.773 | 3.748 | 3.38 | 3.763305e+00 [eV] |
| -0.5 | -4.0 | 5.0 | 3.789 | 3.748 | 3.38 | 3.780310e+00 [eV] |
| -0.9 | -4.0 | 5.0 | 3.823 | 3.748 | 3.38 | 3.813007e+00 [eV] |
| -1.0 | -4.0 | 5.0 | 3.831 | 3.748 | 3.38 | 3.823937e+00 [eV] |
| -1.1 | -4.0 | 5.0 | 3.840 | 3.748 | 3.38 | 3.835696e+00 [eV] |
| -1.3 | -4.0 | 5.0 | 3.856 | 3.748 | 3.38 | 3.861847e+00 [eV] |

| K | U | Hopping | hf H-L gap | TB H-L gap | Exp H-L gap:3.38 | Excitation energy |
|-------|------|---------|------------|------------|------------------|-------------------|
| 4.0 | -1.0 | 4.0 | 3.852 | 3.748 | 3.38 | 3.874466e+00 [eV] |
| 5.0 | -1.0 | 4.0 | 3.831 | 3.748 | 3.38 | 3.823937e+00 [eV] |
| 5.1 | -1.0 | 4.0 | 3.830 | 3.748 | 3.38 | 3.820021e+00 [eV] |
| 5.5 | -1.0 | 4.0 | 3.824 | 3.748 | 3.38 | 3.805833e+00 [eV] |
| 6.0 | -1.0 | 4.0 | 3.817 | 3.748 | 3.38 | 3.790851e+00 [eV] |
| 7.0 | -1.0 | 4.0 | 3.807 | 3.748 | 3.38 | 3.767499e+00 [eV] |
| 8.0 | -1.0 | 4.0 | 3.800 | 3.748 | 3.38 | 3.750126e+00 [eV] |
| 10.0 | -1.0 | 4.0 | 3.789 | 3.748 | 3.38 | 3.726008e+00 [eV] |
| 20.0 | -1.0 | 4.0 | 3.769 | 3.748 | 3.38 | 3.678430e+00 [eV] |
| 100.0 | -1.0 | 4.0 | 3.752 | 3.748 | 3.38 | 3.654311e+00 [eV] |