|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Material | Electronegativity  (eV) | Band gap (eV) | Conduction band bottom (eV) | Valence band top  (eV) |
| Ag2O | 5.29 | 1.20 | -4.69 | -5.89 |
| BaTiO3 | 5.12 | 3.30 | -4.58 | -7.88 |
| Bi2O3 | 6.23 | 2.80 | -4.83 | -7.63 |
| CdO | 5.71 | 2.20 | -4.61 | -6.81 |
| CdFe2O4 | 5.83 | 2.30 | -4.68 | -6.98 |
| Ce2O3 | 5.20 | 2.40 | -4.00 | -6.40 |
| CoO | 5.69 | 2.60 | -4.39 | -6.99 |
| CoTiO3 | 5.76 | 2.25 | -4.64 | -6.89 |
| Cr2O3 | 5.68 | 3.50 | -3.93 | -7.43 |
| CuO | 5.81 | 1.70 | -4.96 | -6.66 |
| Cu2O | 5.32 | 2.20 | -4.22 | -6.42 |
| CuTiO3 | 5.81 | 2.99 | -4.32 | -7.31 |
| FeO | 5.53 | 2.40 | -4.33 | -6.73 |
| Fe2O3 | 5.88 | 2.20 | -4.78 | -6.98 |
| Fe3O4 | 5.78 | 0.10 | -5.73 | -5.83 |
| FeTiO3 | 5.69 | 2.80 | -4.29 | -7.09 |
| Ga2O3 | 5.35 | 4.80 | -2.96 | -7.76 |
| HgO | 6.08 | 1.90 | -5.13 | -7.03 |
| In2O3 | 5.28 | 2.80 | -3.88 | -6.68 |
| KNbO3 | 5.29 | 3.30 | -3.64 | -6.94 |
| KTaO3 | 5.32 | 3.50 | -3.57 | -7.07 |
| La2O3 | 5.28 | 5.50 | -2.53 | -8.03 |
| LiNbO3 | 5.52 | 3.50 | -3.77 | -7.27 |
| LiTaO3 | 5.55 | 4.00 | -3.55 | -7.55 |
| MgTiO3 | 5.60 | 3.70 | -3.75 | -7.45 |
| MnO‘ | 5.29 | 3.60 | -3.49 | -7.09 |
| MnO2 | 5.95 | 0.25 | -5.83 | -6.08 |
| MnTiO3 | 5.59 | 3.10 | -4.04 | -7.14 |
| Nb2O5 | 6.29 | 3.40 | -4.59 | -7.99 |
| NiO | 5.75 | 3.50 | -4.00 | -7.50 |
| NiTiO3 | 5.79 | 2.18 | -4.70 | -6.88 |
| PbO | 5.42 | 2.80 | -4.02 | -6.82 |
| PdO | 579 | 1.00 | -5.29 | -6.29 |
| Sb2O3 | 6.32 | 3.00 | -4.82 | -7.82 |
| SnO | 5.69 | 4.20 | -3.59 | -7.79 |
| SnO2 | 6.25 | 3.50 | -4.50 | -8.00 |
| SrTiO3 | 4.94 | 3.40 | -3.24 | -6.64 |
| Ta2O3 | 6.33 | 4.00 | -4.33 | -8.33 |
| TiO2 | 5.81 | 3.20 | -4.21 | -7.41 |
| V2O5 | 6.10 | 2.80 | -4.70 | -7.50 |
| WO3 | 6.59 | 2.70 | -5.24 | -7.94 |
| ZnO | 5.79 | 3.20 | -4.19 | -7.39 |
| ZnTiO3 | 5.80 | 3.06 | -4.27 | -7.34 |
| ZrO2 | 5.91 | 5.00 | -3.41 | -8.41 |
| Material | Electronegativity (eV) | Band gap (eV) | Conduction band bottom (eV) | Valence band top (eV) |
| Ag2S | 4.96 | 0.92 | -4.50 | -5.42 |
| AS2S3 | 5.83 | 2.50 | -4.58 | -7.08 |
| CdS | 5.18 | 2.40 | -3.98 | -6.38 |
| CoS | 5.17 | 0.00 | -5.17 | -5.17 |
| CoS2 | 5.49 | 0.00 | -5.49 | -5.49 |
| CuS | 5.27 | 0.00 | -5.27 | -5.27 |
| CuS2 | 4.99 | 0.00 | -5.57 | -5.57 |
| CuFeS2 | 5.15 | 0.35 | -4.97 | -5.32 |
| FeS | 5.02 | 0.10 | -4.97 | -5.07 |
| FeS2 | 5.39 | 0.95 | -4.92 | -5.87 |
| In2S3 | 4.70 | 2.00 | -3.70 | -5.70 |
| MnS | 4.81 | 3.00 | -3.31 | -6.31 |
| MnS2 | 5.24 | 0.50 | -4.99 | -5.49 |
| MoS2 | 5.32 | 1.17 | -4.73 | -5.90 |
| NiS | 5.23 | 0.40 | -5.03 | -5.43 |
| NiS2 | 5.54 | 0.30 | -5.39 | -5.69 |
| PbS | 4.92 | 0.37 | -4.74 | -5.11 |
| PbCuSbS3 | 5.22 | 1.23 | --4.61 | -5.84 |
| PtS2 | 6.00 | 0.95 | -5.53 | -6.48 |
| Rh2S3 | 5.36 | 1.50 | -4.61 | -6.11 |
| RuS2 | 5.58 | 1.38 | -4.89 | -6.27 |
| Sb2S3 | 5.63 | 1.72 | -4.72 | -6.44 |
| SnS | 5.17 | 1.01 | -4.66 | -5.67 |
| SnS2 | 5.49 | 2.10 | -4.44 | -6.54 |
| TiS2 | 5.11 | 0.70 | -4.76 | -5.46 |
| WS2 | 5.54 | 1.35 | -4.86 | -6.21 |
| ZnS | 5.26 | 3.60 | -3.46 | -7.06 |
| ZnS2 | 5.56 | 2.70 | -4.21 | -6.91 |
| Zn3In2S6 | 5.00 | 2.81 | -3.59 | -6.40 |
| ZrS2 | 5.20 | 1.82 | -4.29 | -6.11 |

The values are calculated using the following two equations

Ec = -A = -χ +0.5 Eg

Ev = -I =-χ – 0.5 Eg where χ is electronegativity, Eg is the band gap, A is electron affinity and I is theionization potential.