**Table 3:** The IDs, chemical formulas, PBE band gaps and HSE06 band gaps of the screened 114 materials. The predicted HSE06 band gaps of these materials are around 3.0 eV (2.9-3.1 eV), which can be further explored as the superior sensing materials.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| ID | Chemical formula | PBE *E*g (eV) | HSE06 *E*g (eV) | ID | Chemical formula | PBE *E*g (eV) | HSE06 *E*g (eV) |
| N-252 | ZnN6 | 2.90 | 3.08 | S-267 | ZnS | 1.20 | 2.97 |
| N-257 | GaN | 0.01 | 2.94 | S-272 | ZnS | 0.83 | 2.90 |
| N-258 | GaN | 0.09 | 2.94 | S-273 | ZnS | 1.04 | 2.98 |
| N-262 | GaN | 0.08 | 3.02 | S-279 | ZnS | 0.92 | 2.98 |
| N-268 | GaN | 0.09 | 3.02 | S-285 | ZnS | 0.86 | 2.97 |
| N-269 | GaN | 0.16 | 3.07 | S-292 | ZnS | 1.03 | 2.90 |
| N-272 | GaN | 0.02 | 3.07 | S-294 | ZnS | 1.40 | 3.06 |
| N-274 | GaN | 0.00 | 2.95 | S-299 | ZnS | 1.17 | 3.06 |
| N-284 | GaN | 0.04 | 2.92 | S-308 | ZnS | 0.88 | 2.94 |
| N-286 | GaN | 0.05 | 2.93 | S-311 | ZnS | 1.18 | 2.99 |
| N-297 | Ge3N4 | 1.92 | 3.02 | S-315 | ZnS | 1.14 | 3.04 |
| N-298 | Ge3N4 | 1.41 | 3.05 | S-318 | ZnS | 1.25 | 3.06 |
| N-323 | YN | 0.21 | 3.04 | S-320 | ZnS | 0.34 | 3.03 |
| N-450 | CdN6 | 2.78 | 2.96 | S-322 | ZnS | 0.58 | 3.03 |
| N-463 | SbN9 | 2.88 | 3.02 | S-324 | ZnS | 1.22 | 2.93 |
| N-624 | PbN6 | 2.28 | 2.94 | S-325 | ZnS | 0.87 | 2.93 |
| N-629 | BiN | 0.81 | 3.04 | S-328 | ZnS | 0.91 | 2.97 |
| O-1012 | ZrO2 | 3.43 | 3.05 | S-330 | ZnS | 1.28 | 2.99 |
| O-1032 | Nb2O5 | 2.45 | 2.94 | S-336 | ZnS | 1.01 | 3.01 |
| O-1040 | MoO3 | 0.93 | 3.02 | S-339 | ZnS | 0.86 | 2.94 |
| O-1043 | MoO3 | 0.85 | 3.07 | S-340 | ZnS | 0.83 | 2.96 |
| O-1047 | Mo3O10 | 0.34 | 3.02 | S-343 | ZnS | 0.68 | 3.01 |
| O-1052 | MoO3 | 2.00 | 2.92 | S-344 | ZnS | 0.48 | 3.02 |
| O-1063 | MoO3 | 1.85 | 2.98 | S-346 | ZnS | 1.27 | 3.00 |
| O-1069 | MoO3 | 1.65 | 3.04 | S-348 | ZnS | 0.95 | 2.96 |
| O-1085 | MoO3 | 0.50 | 2.99 | S-351 | ZnS | 0.94 | 3.00 |
| O-1090 | MoO3 | 1.37 | 2.94 | S-355 | ZnS | 0.88 | 2.96 |
| O-1131 | Ag2O3 | 0.34 | 2.91 | S-358 | ZnS | 0.93 | 2.93 |
| O-1257 | Cs2O2 | 1.66 | 2.91 | S-360 | ZnS | 0.86 | 2.99 |
| O-1472 | HgO2 | 0.03 | 3.00 | S-367 | ZnS | 1.30 | 3.00 |
| O-1479 | Pb2O3 | 1.07 | 2.94 | S-368 | ZnS | 0.11 | 2.94 |
| O-1488 | PbO2 | 0.02 | 2.90 | S-378 | ZnS | 0.64 | 2.95 |
| O-1497 | Pb2O3 | 0.81 | 3.07 | S-379 | ZnS | 1.42 | 2.95 |
| O-1499 | Pb2O3 | 0.14 | 2.98 | S-381 | ZnS | 0.82 | 2.97 |
| O-350 | V4O7 | 0.09 | 2.96 | S-385 | ZnS | 1.06 | 2.96 |
| O-376 | V2O5 | 1.79 | 2.92 | S-386 | ZnS | 1.36 | 3.05 |
| O-381 | V2O5 | 2.42 | 2.93 | S-388 | ZnS | 1.04 | 2.96 |
| O-389 | V5O12 | 1.08 | 2.94 | S-390 | ZnS | 1.25 | 3.01 |
| O-42 | Na2O | 1.51 | 3.00 | S-394 | ZnS | 0.79 | 3.05 |
| O-58 | MgO | 2.07 | 2.92 | S-403 | Ga2S3 | 1.81 | 3.03 |
| O-593 | Mn2O3 | 0.08 | 3.02 | S-404 | Ga2S3 | 1.70 | 3.09 |
| O-601 | MnO2 | 0.45 | 3.08 | S-415 | RbS | 1.59 | 3.05 |
| O-602 | MnO2 | 1.07 | 3.00 | S-532 | CdS | 0.28 | 3.03 |
| O-605 | MnO2 | 0.90 | 2.94 | S-533 | CdS | 0.28 | 3.06 |
| O-618 | Mn8O17 | 0.31 | 2.91 | S-573 | Sb2S3 | 1.28 | 3.08 |
| O-629 | Mn2O3 | 0.24 | 3.04 | S-578 | CsS | 1.74 | 3.05 |
| O-70 | MgO | 3.00 | 2.98 | S-582 | CsS3 | 1.65 | 2.90 |
| O-72 | MgO | 1.88 | 2.94 | S-583 | BaS | 2.16 | 3.06 |
| O-782 | CoO2 | 0.92 | 3.00 | S-652 | Tl2S | 1.01 | 3.07 |
| O-792 | CoO4 | 0.06 | 2.94 | S-653 | Tl4S3 | 0.86 | 3.10 |
| O-866 | CuO2 | 0.01 | 3.02 | S-654 | TlS | 0.81 | 2.98 |
| O-935 | Rb2O | 0.35 | 2.93 | S-657 | PbS | 0.76 | 3.06 |
| O-943 | Rb2O | 1.32 | 2.99 | S-661 | PbS | 0.75 | 3.01 |
| S-14 | Na2S5 | 1.76 | 2.91 | S-667 | PbS | 1.74 | 3.10 |
| S-259 | ZnS | 0.81 | 3.03 | S-668 | PbS | 1.22 | 3.01 |
| S-260 | ZnS | 0.85 | 2.95 | S-672 | PbS | 1.21 | 3.04 |