**Table 2:** The IDs, chemical formulas, PBE band gaps and HSE06 band gaps of the screened 299 materials. The predicted HSE06 band gaps of these materials are more than 4.0 eV, which provides a brand-new opportunity for using bipolar oxide as switches to manage large amounts of electrical energy, such as in high-power electronics or solar-blind ultraviolet photodetectors.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| ID | Chemical formula | PBE *E*g (eV) | HSE06 *E*g (eV) | ID | Chemical formula | PBE *E*g (eV) | HSE06 *E*g (eV) |
| N-13 | NaN3 | 3.94 | 4.94 | O-143 | Al2O3 | 5.85 | 6.64 |
| N-15 | NaN3 | 0.81 | 4.72 | O-1433 | Re2O7 | 0.05 | 4.98 |
| N-18 | NaN3 | 4.02 | 4.98 | O-1434 | Re2O7 | 3.47 | 4.95 |
| N-24 | NaN3 | 0.87 | 4.28 | O-144 | Al2O3 | 2.73 | 5.70 |
| N-26 | MgN8 | 0.78 | 4.30 | O-145 | Al2O3 | 3.08 | 6.03 |
| N-271 | GaN | 1.10 | 4.77 | O-146 | Al2O3 | 4.22 | 6.37 |
| N-279 | GaN | 0.07 | 4.15 | O-1462 | Au2O3 | 0.82 | 4.43 |
| N-28 | AlN | 4.05 | 4.56 | O-147 | Al2O3 | 2.87 | 5.62 |
| N-293 | GaN | 0.03 | 4.17 | O-148 | Al2O3 | 3.26 | 5.68 |
| N-299 | Ge3N4 | 1.89 | 4.56 | O-149 | Al2O3 | 3.34 | 5.80 |
| N-30 | AlN | 3.33 | 5.17 | O-152 | Al2O3 | 2.76 | 5.69 |
| N-300 | Ge3N4 | 2.06 | 4.31 | O-153 | Al2O3 | 2.66 | 5.68 |
| N-301 | Ge3N2 | 0.53 | 6.08 | O-155 | Al2O3 | 2.81 | 5.67 |
| N-302 | Ge3N4 | 1.61 | 4.47 | O-156 | Al2O3 | 3.33 | 5.63 |
| N-306 | RbN3 | 3.75 | 4.58 | O-157 | Al2O3 | 3.31 | 5.77 |
| N-308 | RbN3 | 4.17 | 4.92 | O-158 | Al2O3 | 3.04 | 5.63 |
| N-312 | Sr2N | 0.04 | 5.80 | O-159 | Al2O3 | 4.01 | 6.00 |
| N-314 | Sr2N | 0.08 | 6.60 | O-160 | Al2O3 | 4.06 | 6.07 |
| N-316 | Sr3N2 | 0.35 | 5.54 | O-161 | Al2O3 | 2.97 | 5.84 |
| N-32 | KN3 | 4.16 | 4.29 | O-162 | Al2O3 | 4.66 | 5.66 |
| N-322 | Sr4N3 | 0.02 | 5.19 | O-163 | Al2O3 | 3.35 | 5.64 |
| N-326 | YN | 2.09 | 5.94 | O-164 | Al2O3 | 5.66 | 6.06 |
| N-455 | InN | 0.00 | 7.37 | O-165 | Al2O3 | 2.93 | 5.83 |
| N-460 | SbN | 0.07 | 5.33 | O-167 | Al2O3 | 2.89 | 5.57 |
| N-461 | SbN | 0.30 | 5.30 | O-168 | Al2O3 | 4.60 | 6.04 |
| N-462 | SbN | 0.30 | 5.27 | O-169 | Al2O3 | 3.00 | 5.71 |
| N-464 | SbN | 0.17 | 5.34 | O-170 | Al2O3 | 4.24 | 5.60 |
| N-465 | SbN | 0.09 | 5.41 | O-171 | Al2O3 | 2.85 | 5.62 |
| N-467 | CsN2 | 0.05 | 5.45 | O-172 | Al2O3 | 4.81 | 5.17 |
| N-469 | CsN3 | 4.22 | 5.04 | O-173 | Al2O3 | 3.39 | 5.51 |
| N-470 | Ba3N2 | 0.11 | 5.52 | O-174 | Al2O3 | 4.00 | 5.67 |
| N-471 | Ba2N | 0.05 | 6.48 | O-176 | Al2O3 | 2.87 | 5.72 |
| N-52 | ScN | 2.45 | 5.68 | O-177 | Al2O3 | 2.72 | 5.76 |
| N-536 | WN6 | 0.36 | 4.36 | O-179 | Al2O3 | 1.36 | 5.61 |
| O-100 | Al2O3 | 3.30 | 5.79 | O-180 | Al2O3 | 4.46 | 6.24 |
| O-1000 | ZrO2 | 3.87 | 4.40 | O-181 | AlO2 | 1.09 | 5.58 |
| O-1003 | ZrO2 | 2.87 | 4.14 | O-185 | KO3 | 0.84 | 4.05 |
| O-1006 | ZrO2 | 3.96 | 4.27 | O-194 | KO2 | 0.50 | 4.87 |
| O-1007 | ZrO2 | 2.86 | 5.17 | O-199 | K2O | 0.65 | 4.09 |
| O-101 | Al2O3 | 3.13 | 5.80 | O-218 | ScO2 | 0.46 | 4.49 |
| O-1011 | Zr19O40 | 0.04 | 4.36 | O-219 | Sc2O3 | 3.82 | 6.61 |
| O-1013 | ZrO2 | 3.86 | 4.28 | O-220 | Sc2O3 | 4.05 | 5.88 |
| O-1014 | ZrO2 | 3.47 | 4.02 | O-221 | Sc2O3 | 3.48 | 6.72 |
| O-102 | Al2O3 | 3.18 | 5.74 | O-225 | Sc2O3 | 3.41 | 7.85 |
| O-103 | AlO2 | 0.07 | 5.05 | O-228 | ScO2 | 0.57 | 5.06 |
| O-104 | Al2O3 | 3.00 | 5.80 | O-229 | Sc2O3 | 4.14 | 5.35 |
| O-105 | Al2O3 | 2.97 | 5.73 | O-230 | Sc2O3 | 4.16 | 5.82 |
| O-108 | Al2O3 | 2.67 | 5.65 | O-238 | TiO2 | 2.84 | 4.20 |
| O-109 | Al2O3 | 3.48 | 5.68 | O-245 | TiO2 | 2.41 | 4.10 |
| O-110 | Al2O3 | 3.39 | 5.59 | O-247 | Ti3O7 | 0.15 | 4.10 |
| O-111 | Al2O3 | 4.17 | 6.41 | O-250 | TiO2 | 3.45 | 4.72 |
| O-112 | Al2O3 | 3.11 | 5.98 | O-253 | Ti3O5 | 0.01 | 4.04 |
| O-113 | Al2O3 | 3.46 | 5.60 | O-263 | Ti3O5 | 0.02 | 4.10 |
| O-114 | Al2O3 | 2.78 | 5.82 | O-277 | TiO2 | 2.57 | 4.16 |
| O-1145 | CdO | 0.01 | 4.14 | O-281 | TiO2 | 3.31 | 4.38 |
| O-1147 | In2O3 | 0.68 | 8.25 | O-294 | TiO2 | 2.98 | 4.02 |
| O-1148 | In2O3 | 0.89 | 7.96 | O-300 | TiO2 | 2.77 | 4.20 |
| O-1149 | In2O3 | 0.77 | 7.78 | O-302 | TiO2 | 1.07 | 4.03 |
| O-1150 | In2O3 | 0.67 | 8.23 | O-306 | TiO2 | 1.70 | 4.10 |
| O-1151 | In2O3 | 0.11 | 9.21 | O-334 | Ti2O7 | 1.15 | 4.19 |
| O-1152 | In2O3 | 0.96 | 8.17 | O-600 | MnO2 | 1.15 | 5.54 |
| O-1155 | InO2 | 0.27 | 5.41 | O-61 | MgO | 2.26 | 4.63 |
| O-1156 | In2O3 | 0.93 | 9.97 | O-742 | FeO | 0.86 | 5.36 |
| O-1157 | In2O3 | 0.21 | 8.88 | O-82 | Al2O3 | 3.29 | 5.71 |
| O-1158 | SnO | 0.48 | 5.96 | O-84 | Al2O3 | 3.39 | 5.73 |
| O-1159 | SnO | 0.52 | 5.87 | O-85 | Al2O3 | 3.25 | 5.85 |
| O-116 | Al2O3 | 3.14 | 5.69 | O-88 | Al2O3 | 4.83 | 6.01 |
| O-1160 | SnO | 0.54 | 5.47 | O-895 | ZnO | 0.74 | 4.06 |
| O-1161 | SnO2 | 2.00 | 4.43 | O-899 | ZnO | 0.45 | 4.32 |
| O-1162 | SnO2 | 0.79 | 5.25 | O-90 | Al2O3 | 3.77 | 6.10 |
| O-1163 | SnO2 | 0.26 | 4.57 | O-904 | Ga2O3 | 1.29 | 4.52 |
| O-1164 | SnO | 0.02 | 5.95 | O-907 | Ga2O3 | 2.41 | 4.05 |
| O-1166 | SnO2 | 1.05 | 4.29 | O-908 | Ga2O3 | 1.20 | 4.09 |
| O-1167 | SnO | 1.49 | 6.01 | O-909 | Ga2O3 | 1.38 | 4.61 |
| O-1169 | SnO2 | 0.32 | 4.64 | O-914 | Ga2O3 | 1.04 | 4.51 |
| O-117 | Al2O3 | 5.49 | 6.06 | O-915 | Ga2O3 | 1.27 | 4.53 |
| O-1170 | SnO | 0.53 | 5.96 | O-916 | Ga2O3 | 1.31 | 4.54 |
| O-1173 | SnO2 | 0.43 | 4.65 | O-917 | GeO2 | 1.37 | 5.31 |
| O-1177 | SnO | 1.43 | 5.88 | O-919 | GeO2 | 3.28 | 6.38 |
| O-1178 | SnO2 | 0.06 | 4.57 | O-92 | Al2O3 | 3.08 | 5.55 |
| O-1179 | SnO2 | 0.57 | 4.78 | O-921 | Ge2O3 | 0.70 | 5.63 |
| O-118 | Al2O3 | 3.28 | 5.71 | O-922 | GeO2 | 2.95 | 6.07 |
| O-1180 | SnO2 | 0.57 | 4.62 | O-923 | GeO2 | 0.97 | 4.39 |
| O-1182 | SnO | 0.41 | 5.49 | O-924 | GeO2 | 1.23 | 5.29 |
| O-1184 | Sn5O6 | 1.76 | 5.18 | O-925 | GeO2 | 3.25 | 6.31 |
| O-1185 | SnO2 | 2.09 | 4.04 | O-926 | GeO2 | 0.78 | 4.68 |
| O-1189 | SnO2 | 0.70 | 4.69 | O-928 | GeO2 | 3.25 | 6.29 |
| O-119 | Al2O3 | 3.21 | 5.70 | O-929 | GeO2 | 1.52 | 5.31 |
| O-1191 | SnO2 | 1.76 | 4.14 | O-93 | Al2O3 | 2.90 | 5.54 |
| O-1193 | SnO2 | 0.36 | 4.70 | O-938 | Rb16O3 | 0.09 | 4.60 |
| O-1194 | SnO2 | 1.33 | 4.59 | O-94 | Al2O3 | 5.44 | 6.03 |
| O-1196 | Sn5O7 | 0.38 | 4.94 | O-95 | Al2O3 | 3.19 | 5.74 |
| O-1198 | SnO2 | 2.09 | 4.20 | O-951 | SrO | 2.94 | 4.30 |
| O-1199 | SnO2 | 0.41 | 4.00 | O-954 | SrO10 | 0.31 | 4.06 |
| O-120 | Al2O3 | 0.69 | 6.06 | O-955 | SrO2 | 2.86 | 4.46 |
| O-1201 | SnO2 | 2.09 | 4.41 | O-956 | SrO | 2.56 | 4.64 |
| O-1202 | SnO2 | 1.59 | 4.21 | O-959 | SrO4 | 0.30 | 8.17 |
| O-1209 | Sb2O3 | 2.22 | 4.20 | O-96 | AlO2 | 0.33 | 5.08 |
| O-121 | Al2O3 | 1.99 | 5.62 | O-965 | SrO | 3.29 | 4.99 |
| O-122 | Al2O3 | 3.35 | 5.83 | O-968 | YO2 | 0.28 | 5.05 |
| O-1225 | SbO2 | 1.85 | 4.23 | O-969 | Y2O3 | 4.44 | 4.55 |
| O-1230 | Sb2O3 | 2.35 | 4.28 | O-97 | Al2O3 | 3.13 | 5.72 |
| O-1231 | Sb2O3 | 2.55 | 4.41 | O-971 | Y2O3 | 2.80 | 4.70 |
| O-1232 | Sb2O3 | 1.22 | 4.02 | O-972 | Y2O3 | 1.58 | 5.41 |
| O-1239 | Sb2O3 | 1.22 | 4.11 | O-973 | Y2O3 | 3.57 | 4.57 |
| O-124 | Al2O3 | 3.62 | 5.57 | O-974 | Y2O3 | 3.96 | 4.65 |
| O-1240 | SbO2 | 1.33 | 4.02 | O-975 | Y2O3 | 2.91 | 4.56 |
| O-1246 | SbO2 | 2.40 | 4.05 | O-976 | Y2O3 | 2.82 | 4.65 |
| O-125 | Al2O3 | 2.66 | 5.74 | O-977 | Y2O3 | 4.10 | 4.94 |
| O-126 | Al2O3 | 3.51 | 5.81 | O-979 | Y2O3 | 3.05 | 4.62 |
| O-1265 | BaO | 1.77 | 4.69 | O-98 | Al2O3 | 5.31 | 5.53 |
| O-1267 | BaO6 | 0.02 | 4.14 | O-981 | Y2O3 | 4.06 | 4.83 |
| O-1274 | BaO | 2.30 | 4.04 | O-982 | Y2O3 | 4.39 | 4.46 |
| O-1275 | BaO | 2.15 | 5.46 | O-984 | Y2O3 | 2.94 | 4.61 |
| O-1277 | BaO | 2.37 | 4.11 | O-985 | ZrO2 | 3.72 | 4.24 |
| O-1279 | BaO | 1.70 | 4.72 | O-99 | Al2O3 | 4.37 | 5.70 |
| O-1281 | BaO | 2.77 | 4.67 | O-992 | ZrO2 | 3.21 | 4.10 |
| O-1283 | BaO | 1.75 | 4.64 | O-993 | ZrO2 | 3.13 | 4.73 |
| O-1284 | BaO | 1.30 | 4.70 | O-994 | Zr6O11 | 0.37 | 4.40 |
| O-1287 | BaO | 1.48 | 4.89 | O-996 | ZrO2 | 3.31 | 4.61 |
| O-1288 | BaO2 | 3.66 | 4.13 | O-998 | ZrO2 | 4.20 | 4.02 |
| O-1289 | HfO2 | 3.40 | 4.22 | S-33 | Al2S3 | 1.04 | 4.40 |
| O-129 | Al2O3 | 5.22 | 5.38 | S-398 | GaS | 1.86 | 4.02 |
| O-1290 | HfO2 | 3.39 | 4.29 | S-399 | GaS | 1.88 | 4.01 |
| O-1291 | HfO2 | 3.62 | 4.18 | S-401 | GaS | 2.01 | 4.01 |
| O-1292 | HfO2 | 3.82 | 4.84 | S-424 | Rb2S | 1.89 | 4.19 |
| O-1294 | HfO2 | 3.77 | 4.12 | S-44 | KS | 0.39 | 5.02 |
| O-1295 | HfO2 | 3.48 | 4.16 | S-535 | CdS | 1.12 | 4.57 |
| O-1298 | HfO2 | 4.02 | 4.11 | S-536 | CdS | 1.05 | 4.58 |
| O-130 | Al2O3 | 4.27 | 6.09 | S-537 | CdS | 1.52 | 4.30 |
| O-1300 | HfO2 | 3.75 | 4.13 | S-540 | In2S3 | 0.83 | 4.10 |
| O-1302 | HfO2 | 4.67 | 4.48 | S-541 | In2S3 | 0.29 | 4.20 |
| O-1303 | HfO2 | 4.02 | 4.09 | S-543 | In6S7 | 0.32 | 4.51 |
| O-1304 | Ta2O5 | 2.96 | 4.61 | S-544 | In2S3 | 0.49 | 4.53 |
| O-1305 | Ta2O5 | 3.15 | 4.08 | S-546 | InS | 1.38 | 5.14 |
| O-1311 | Ta2O5 | 3.30 | 4.13 | S-548 | InS | 0.37 | 5.46 |
| O-1313 | Ta2O5 | 1.66 | 4.79 | S-551 | In2S3 | 0.82 | 5.30 |
| O-1318 | Ta2O5 | 2.57 | 4.01 | S-553 | In2S3 | 1.09 | 5.10 |
| O-1326 | TaO2 | 0.77 | 4.07 | S-560 | SnS | 1.47 | 4.29 |
| O-133 | Al2O3 | 2.99 | 5.77 | S-561 | SnS | 1.18 | 4.13 |
| O-1334 | Ta2O5 | 3.89 | 4.20 | S-562 | SnS | 0.06 | 4.09 |
| O-134 | Al2O3 | 3.44 | 5.49 | S-565 | SnS | 0.20 | 4.60 |
| O-136 | Al2O3 | 1.64 | 5.66 | S-566 | SnS | 0.95 | 4.17 |
| O-137 | Al2O3 | 2.99 | 5.49 | S-567 | SnS | 1.59 | 4.26 |
| O-138 | Al2O3 | 3.05 | 5.89 | S-569 | SnS | 1.43 | 4.02 |
| O-139 | Al2O3 | 3.97 | 5.63 | S-634 | Au2S | 1.90 | 4.60 |
| O-140 | Al2O3 | 2.58 | 5.68 | S-638 | HgS4 | 1.05 | 6.12 |
| O-141 | Al2O3 | 3.29 | 5.72 | S-81 | TiS | 0.80 | 4.08 |
| O-142 | Al2O3 | 2.94 | 5.67 |  |  |  |  |