**Table 1:** The IDs, chemical formulas, PBE band gaps and HSE06 band gaps of the screened 33 materials. The predicted HSE06 band gaps of these materials are less than 0.9 eV, which may be promising electrode and electrocatalytic materials with high electronic conductivities.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| ID | Chemical formula | PBE *E*g (eV) | HSE06 *E*g (eV) | ID | Chemical formula | PBE *E*g (eV) | HSE06 *E*g (eV) |
| N-485 | HfN2 | 0.59 | 0.90 | O-695 | Fe3O4 | 0.80 | 0.48 |
| N-486 | Hf3N4 | 1.03 | 0.84 | O-705 | Fe2O3 | 1.16 | 0.45 |
| N-522 | WN2 | 0.57 | 0.71 | O-714 | Fe2O3 | 0.94 | 0.85 |
| N-532 | WN2 | 1.13 | 0.10 | O-720 | Fe4O5 | 1.00 | 0.04 |
| N-543 | WN2 | 1.58 | 0.09 | O-721 | FeO | 1.27 | 0.04 |
| O-644 | FeO | 0.44 | 0.07 | O-725 | FeO | 0.05 | 0.41 |
| O-646 | Fe3O4 | 0.24 | 0.40 | O-726 | Fe3O4 | 0.52 | 0.47 |
| O-650 | Fe3O4 | 0.37 | 0.79 | O-729 | Fe3O4 | 0.98 | 0.39 |
| O-659 | Fe3O4 | 0.93 | 0.42 | O-737 | Fe23O32 | 0.63 | 0.67 |
| O-671 | Fe3O4 | 0.01 | 0.38 | O-748 | Fe2O3 | 1.52 | 0.71 |
| O-679 | Fe2O3 | 1.53 | 0.45 | O-750 | Fe3O4 | 0.55 | 0.02 |
| O-683 | Fe3O4 | 0.82 | 0.49 | O-756 | Fe3O4 | 0.88 | 0.48 |
| O-686 | Fe2O3 | 0.63 | 0.53 | O-762 | Fe3O4 | 0.49 | 0.48 |
| O-688 | Fe15O16 | 1.34 | 0.39 | O-764 | Fe2O3 | 0.66 | 0.35 |
| O-690 | FeO | 0.20 | 0.45 | O-765 | Fe5O7 | 1.13 | 0.34 |
| O-691 | Fe3O4 | 0.74 | 0.53 | O-860 | Cu2O | 0.50 | 0.56 |
| O-692 | Fe2O3 | 0.82 | 0.84 |  |  |  |  |