| **Abbreviation** | **Full Name** |
| --- | --- |
| μ | Dipole moment |
| χ | Electronegativity |
| Eg | Band gap |
| t | Tolerance factor |
| θ | Average lattice angle |
| Vcell | Lattice volume |
| dlayer | Spacing of layers |
| Eb | Excitonic binding energy |
| ro | Organic molecular radius |
| α | Polarizability |
| nlayers | Number of layers |
| L | Average lattice parameters |
| dPb–I | Pb–I distance |
| LSF t1 | Layer Stacking Factor t1 |
| LSF t2 | Layer Stacking Factor t2 |
| ELUMO | LUMO energy |
| MW | Average molecular weight (Mass) |
| ΔEH–L | HOMO–LUMO gap |
| EHOMO | HOMO energy |