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Organic Materials Database: Electronic Structure Database with Focus on Data Mining[1] STANISLAV BORYSOV, MATTHIAS GEILHUFE, ALEXANDER BALATSKY, Nordita, Center for Quantum Materials, KTH Royal Institute of Technology and Stockholm University, Roslagstullsbacken 23, SE-106 91 Stockholm, Sweden — We present the Organic Materials Database (OMDB) hosting electronic band structure calculations for thousands of organic and organometallic materials. The electronic band structures are calculated using density functional theory for the crystal structures contained within the Crystallography Open Database. Although these materials were previously synthesized, little attention has been paid to their electronic properties. The OMDB database is freely accessible online at http://omdb.diracmaterials.org. The OMDB web interface allows for identifying materials with certain target band structure and density of states properties specified by the user. We illustrate the use of OMDB and how it can become an organic part of search and prediction of novel functional materials via data mining techniques.

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