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Addition/Correction

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Addition to Crystallographic Information Resources

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A description of the principal available crystallographic databases, both academic/commercial and free, has recently been published as "Crystallographic Information Resources".[1] These databases generally focus on experimental values. I wish now to add an important free database of theoretical crystallographic values,[2] the "Materials Project",[3] which also provides users with a calculational resource for ionic materials using density functional theory. This resource is based upon supercomputing clusters at the Lawrence Berkeley National Laboratory's NERSC Scientific Computing Center and Computational Research Division. The database contains nearly 70,000 ionic structures and over 20,000 molecules as well as much data on the physical properties of the materials.

REFERENCES

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