

Materials Research Science and Engineering Centers

Magnetic Stoichiometric Topological Materials

Magnetic Material Database:

- 500 (soon 1000) interacting magnetic materials
- Axion insulators, semimetals, etc.
- Theory now used in characterization of twisted bilayer graphene, other moire compounds

Topological Magnetic Materials Database

Back to Search Results

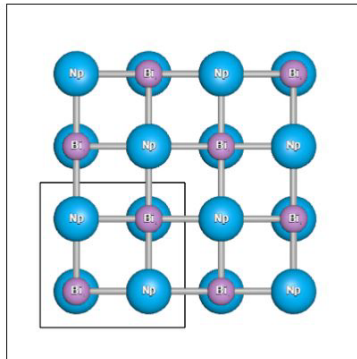
Compound: Np Bi
 Magnetic Symmetry Group: $Pm\bar{3}m'$ (224.113)
 BCS-ID: 3.7

Materials Data

Crystallographic data

Cell Length A	6.37
Cell Length B	6.37
Cell Length C	6.37
Cell Angle α	90
Cell Angle β	90
Cell Angle γ	90

Lattice Structure



Possible Topological Status (Types)

U=0.0	TI
U=2.0	TI
U=4.0	TI
U=6.0	TI

U=0.0 Type: TI

Magnetic moments (μ_B):

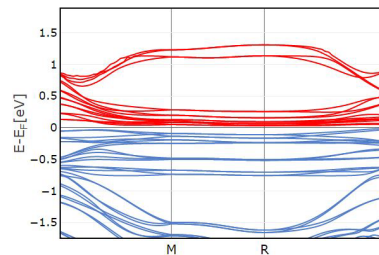
Atom	Position	Exp. μ	Theo. μ	Error (%)
Np	(0.0,0.0,0.0)	(1.4,1.4,1.4)	(2.079,2.082,2.059)	48.05
Np	(0.5,0.5,0.0)	(-1.4,-1.4,1.4)	(-2.077,-2.079,2.058)	47.95
Np	(0.5,0.0,0.5)	(-1.4,1.4,-1.4)	(-2.081,2.082,-2.066)	48.31
Np	(0.0,0.5,0.5)	(1.4,-1.4,-1.4)	(2.079,-2.081,-2.065)	48.22

Average Error = 48.0%

- All magnetic group theory derived and tabulated for 1651 groups
- Topological indices calculated for 1651 groups, physical meaning obtained
- All data is on Bilbao Crystallographic Server

L. Elcoro, B.J. Wieder, Z. Song, Y. Xu, B. Bradlyn, B.A. Bernevig, "Magnetic topological quantum chemistry," *Nature Comm.* **12**, 5965 (2021)

Band Structure



Topological Quantum Chemistry

BANDREP

Band representations and Elementary Band representations of Double Space Groups

Check Topological Mat

Check if a given non-magnetic material is topological or not

MBANDREP

Band corepresentations and Elementary Band corepresentations of Magnetic Double Space Groups

Check Topological Magnetic Mat.

Identify topological materials in magnetic compounds

FragileRoots

Lists of fragile roots in the space groups