Automatic Data Report

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1 Computation resume

The electronic band strucutre was computed with Empirical Pseudopotential Method (EPM).

The following options were used:

• Method: EPM

• Number nearest neighbors: 6

• Number of bands: 6

• Number of kpoints: 2000

• path: LKWGXWLGK

• Nonlocal Correction: Yes

• Spin Orbit Coupling: No