

Energy versus K-points and energy cutoff

Energy cutoff (eV)

300

450

600

750

900

1050

1200

-88.5

-89.0

-89.5

-90.0

-90.5

Energy (eV)

- Energy versus K-points for B₁₄ (ENCUT=450)
- Energy versus K-points for B₁₄ (ENCUT=480)
- Energy versus energy cutoff for B₁₄ (Kpoints:10,14,9)
- Energy versus energy cutoff for B₁₄ (Kpoints:19,27,17)

(4, 6, 4)
(5, 7, 5)
(6, 8, 6)
(7, 10, 6)
(8, 11, 7)
(9, 13, 8)
(10, 14, 9)
(11, 15, 10)
(12, 17, 11)
(13, 18, 12)
(14, 20, 13)
(15, 21, 14)
(16, 23, 15)
(17, 24, 16)
(18, 25, 17)
(19, 27, 17)
(20, 28, 18)
(21, 30, 19)
(22, 31, 20)
(23, 32, 21)
(24, 34, 22)

K-points configuration