

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

-90.5

-90.5

- 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)

Energy (eV)

(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

