Title: DFT study of stepped 4H-SiC{0001} surfaces

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- We presented results of DFT simulations of atomic steps appearing on the 4H-SiC{0001} surfaces in the directions [11-20] and [10-10].
- Calculated ledge energy allowed to identify [11-20] step with C atom on the edge at Si(0001) as the most favourable energetically of all examined cases.
- At C-terminated surface such structures are preferable where C-C bonds can be created and Si is the edge atom.
- On the C-terminated surface atomic and electronic structure is modified only in the nearest vicinity of the edge whereas the structure of the terrace is very close to that of the perfect surface.
- On the Si-terminated surface for both types of the steps considered and on the widest terraces a substantial surface buckling and electronic transfer among Si atoms from the topmost layer are observed in the regions between steps.