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The crystalline Si3N4/Si interface; the electronic structure of defects ESPEN FLAGE-LARSEN, ESPEN SAGVOLDEN, OLE MARTIN LOEVVIK, DAN MICHAEL OLSEN HEGGOE, JESPER FRIIS, SINTEF Materials and Chemistry, P.O. Box 124 Blindern, Forskningsveien 1, N-0314 Oslo, Norway, CHANG-MING FANG, University of Vienna, Faculty of Physics and Center for Computational Materials Science, Sensengasse 8/12, A-1090 Vienna, Austria — A semiconducting beta-Si3N4(0001)/Si(111) interface model without dangling bonds is presented, and its geometric and electronic structure is compared to previous models based on calculations in a density functional theory framework. Furthermore nitrogen and phosphorus defects in the silicon layer are investigated, in particular how these defects modify the electronic structure and the electronic properties of the interface as a function of their distance to it. The local geometric structure of the nitrogen and phosphorus defects is also investigated close to the interface.

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