Title:	First-principles investigation of BaFe2As2(001)
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Abstract:	The structural, electronic, and magnetic properties of several different terminations of the BaFe2As2(001) surface are investigated by means of first-principles calculations. Analysis of the surface stability as a function of the chemical potentials reveals that the three possible terminations (As, full and half Ba coverage) can all be stabilized in different chemical-potential ranges. We determine the most stable structure in each case and study its magnetic and electronic properties. A study of the scanning tunnel microscope maps and work functions provides helpful insights for the interpretation of the still debated experimental findings.