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(1x2) Surface Reconstruction for $Ca(Fe_{1-x}Co_x)_2As_2$: Spin-Charge-Lattice-Coupling[1] GUORONG LI, Dept. of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, LIANGBO LIANG, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, New York 12180, V.B. NASCIMENTO, XIAOBO HE, A.B. KARKI, YIMIN XIONG, Dept. of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, VINCENT MEUNIER, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, New York 12180, RONGYING JIN, JIANDI ZHANG, E.W. PLUMMER, Dept. of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803 — Low energy electron diffraction (LEED) and density functional theory (DFT) have been utilized to investigate the surface structure for the stripe 1x2 phase of $Ca(Fe_{1-x}Co_x)_2As_2$ iron pnictides, for x = 0 and x = 0.075. Quantitative structural analysis of LEED-I(V) using the fractional spots of the 1x2 phase on both parent and doped samples gives a similar surface structure with a termination layer of half Ca atoms. The surface Ca layer has a large inward relaxation about 0.5 Angstrom and the underneath As-Fe-As layer displays a buckling distortion of about 0.07 Angstrom. DFT calculations show significant charge rearrangements at the surface, which is driven by spin charge coupling, verified by freezing the structure and reducing the magnetic moment to zero. The role of spin-charge coupling in determining the surface reconstruction will be elucidated by self-consistent calculations of the structure as a function of the magnetic moment.

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