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The search for stable sp2 zigzag edge graphene nanoribbon termination CHENGING CHIA, VINCENT CRESPI, Department of Physics, Penn State University — The zig-zag edge of a graphene ribbon has attracted much attention, since it is predicted to support a spin-polarized edge state. However, it is difficult to produce thermodynamic conditions that favor a pure sp^2 termination of a graphene sheet, since the edge carbons generally prefer to bond to two hydrogen atoms, in sp^3 hybridization, rather than one hydrogen, as sp^2. We examine several candidate alternative termination groups which can modify the thermodynamics of various edge configurations to favor the sp^2 edge termination. Ab-initio calculations demonstrate these alternative terminations can support robust edge states across a broad range of synthetic conditions.

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