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**Inducing extended line defects in graphene by linear adsorption of C and N atoms** YU LI, RUIQIN ZHANG, City University of Hong Kong, ZIJING LIN, University of Science and Technology of China, MICHEL A. VAN HOVE, Hong Kong Baptist University, USTC-CITYU JOINT ADVANCED RESEARCH CENTRE, SUZHOU 215123, CHINA COLLABORATION, INSITITUTE OF COMPUTATIONAL AND THEORETICAL STUDIES, HONG KONG BAPTIST UNIVERSITY COLLABORATION, GROUP OF RUI-QIN ZHANG TEAM — We propose a possible approach for controlled formation of various 585 (containing pentagonal and octagonal carbon rings) extended line defects (ELDs) by linear adsorption of various kinds of atoms (C, N, B, O) on a graphene substrate, based upon density functional theory and molecular-dynamics (MD) simulations. We find out that the C and N atoms spontaneously transform to 585 ELDs while other elements find specific stable configurations. To confirm the feasibility of forming the ELD from line adsorption, investigation of the critical transformation conditions of the 585 ELD is involved based upon various adsorption models and adsorption densities.

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