

Doping-mediated electronic and magnetic properties of graphene-like ionic NaX (X = F and Cl) monolayers

Bich Ngoc Nguyen Thi,¹ Chu Viet Ha,² Nghiem Thi Ha Lien,³ J. Guerrero-Sanchez,⁴ and D. M. Hoat^{5,6,*}

¹Institute of Physics, Vietnam Academy of Science and Technology, 18 Hoang Quoc Viet, Cau Giay, Hanoi, Vietnam

²Faculty of Physics, TNU-University of Education, Thai Nguyen, 250000, Vietnam

³Institute of Physics, Vietnam Academy of Science and Technology, 10 Dao Tan, Ba Dinh, Hanoi, Vietnam

⁴Universidad Nacional Autónoma de México, Centro de Nanociencias y Nanotecnología, Apartado Postal 14, Ensenada, Baja California, Código Postal 22800, Mexico

⁵Institute of Theoretical and Applied Research, Duy Tan University, Ha Noi 100000, Viet Nam

⁶Faculty of Natural Sciences, Duy Tan University, Da Nang 550000, Viet Nam

*Corresponding author: dominhhoat@duytan.edu.vn

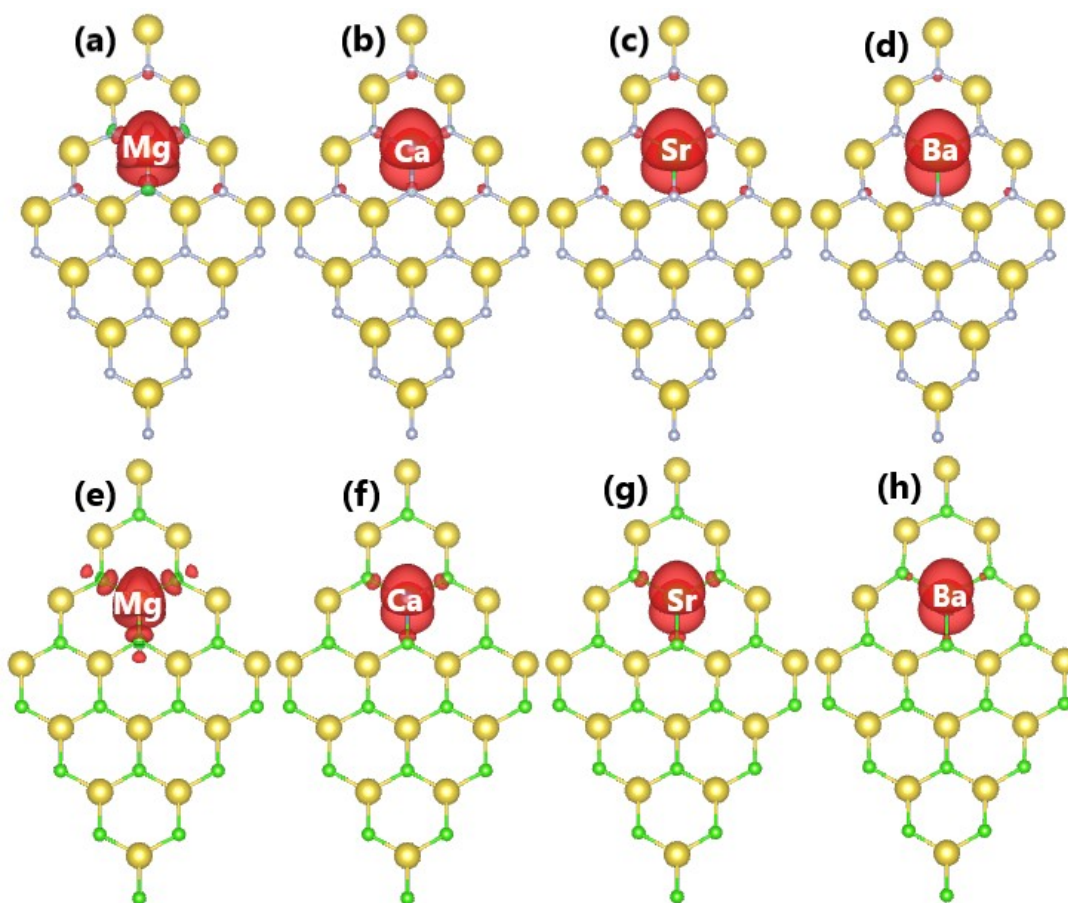


Figure S1: Figure 6. Spin density (Iso-surface value: $0.001 e/\text{\AA}^3$; Na: yellow ball; F: grey ball; Cl: green ball) in NaF monolayer doped with (a) Mg, (b) Ca, (c) Sr, and (d) Ba; and NaCl monolayer doped with (e) Mg, (f) Ca, (g) Sr, and (h) Ba.

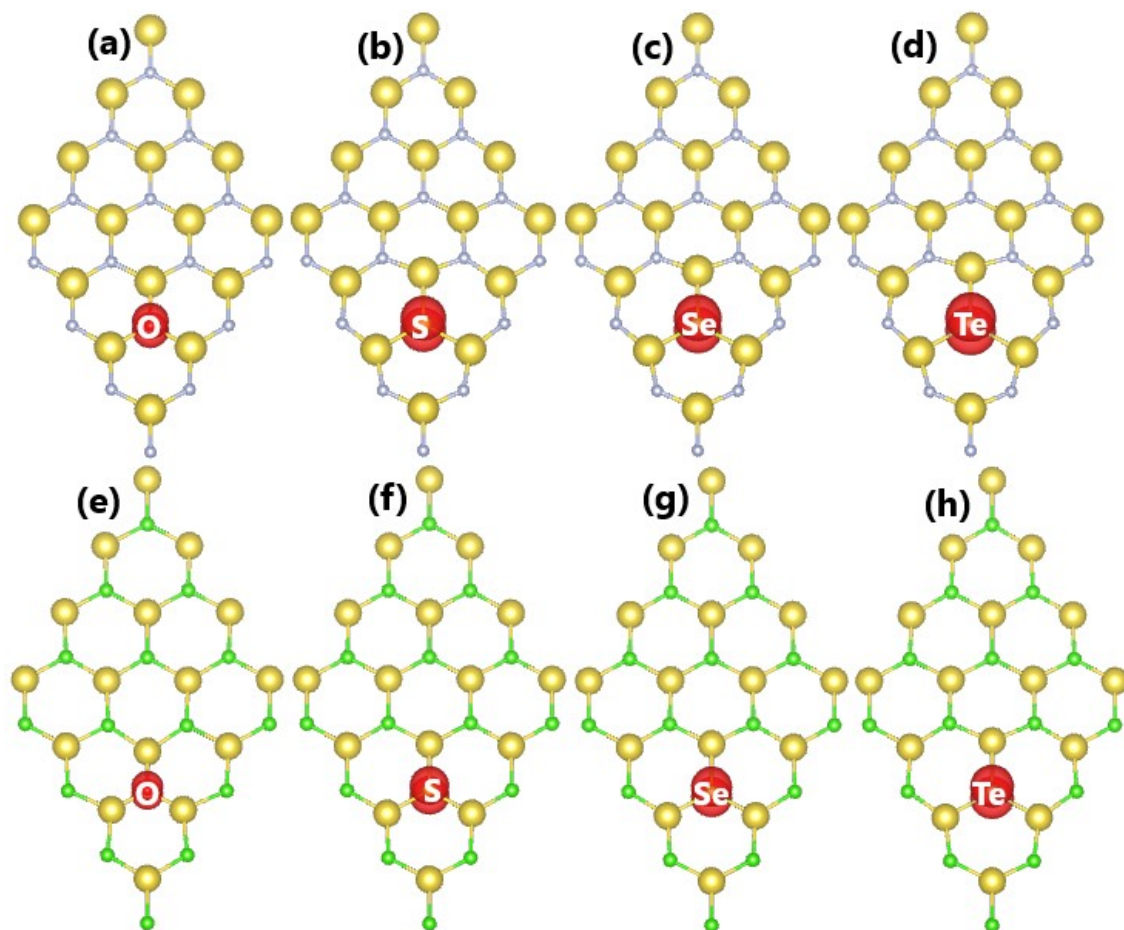


Figure S2: Figure 10. Spin density (Iso-surface value: $0.004 e/\text{\AA}^3$; Na: yellow ball; F: grey ball; Cl: green ball) in NaF monolayer doped with (a) O, (b) S, (c) Se, and (d) Te; and NaCl monolayer doped with (e) O, (f) S, (g) Se, and (h) Te.

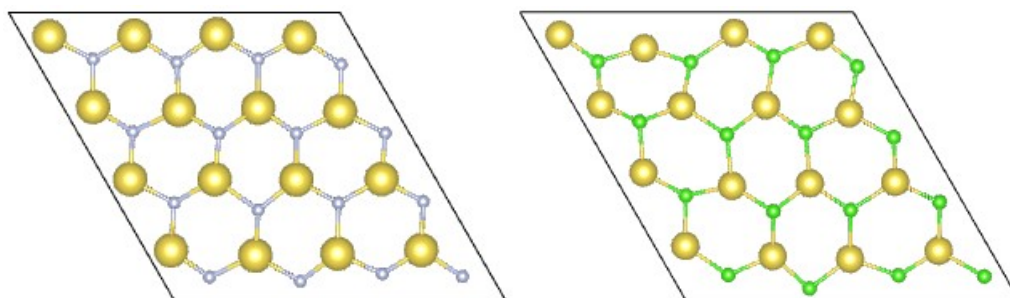


Fig.S3: Atomic structure of NaF (left side) and NaCl (right side) monolayer after 5000 fs of AIMD simulations.

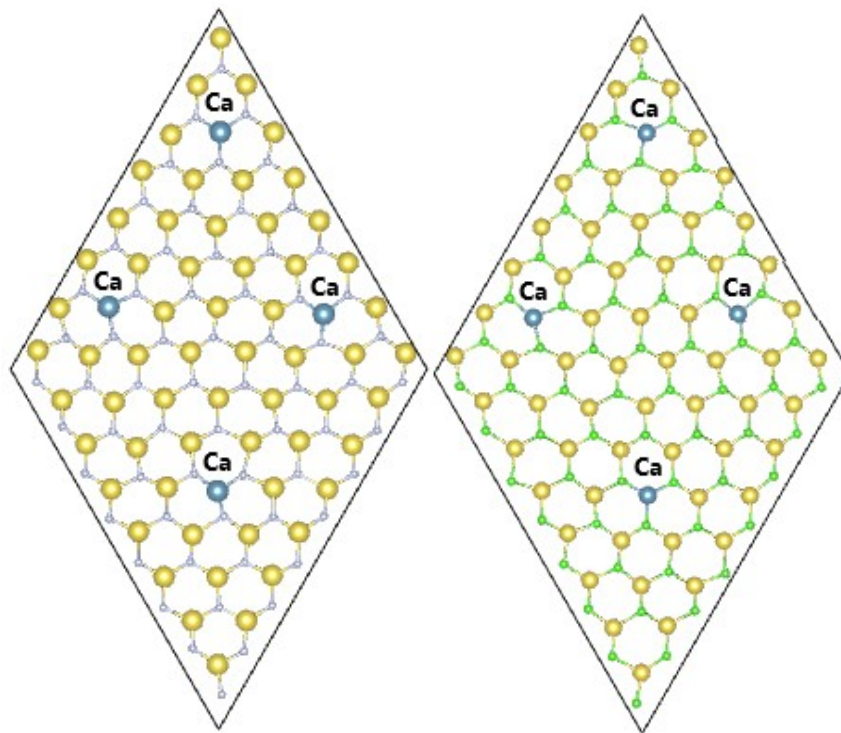


Fig.S3 (cont): Atomic structure of Ca-doped NaF (left side) and Ca-doped NaCl (right side) monolayer after 5000 fs of AIMD simulations.

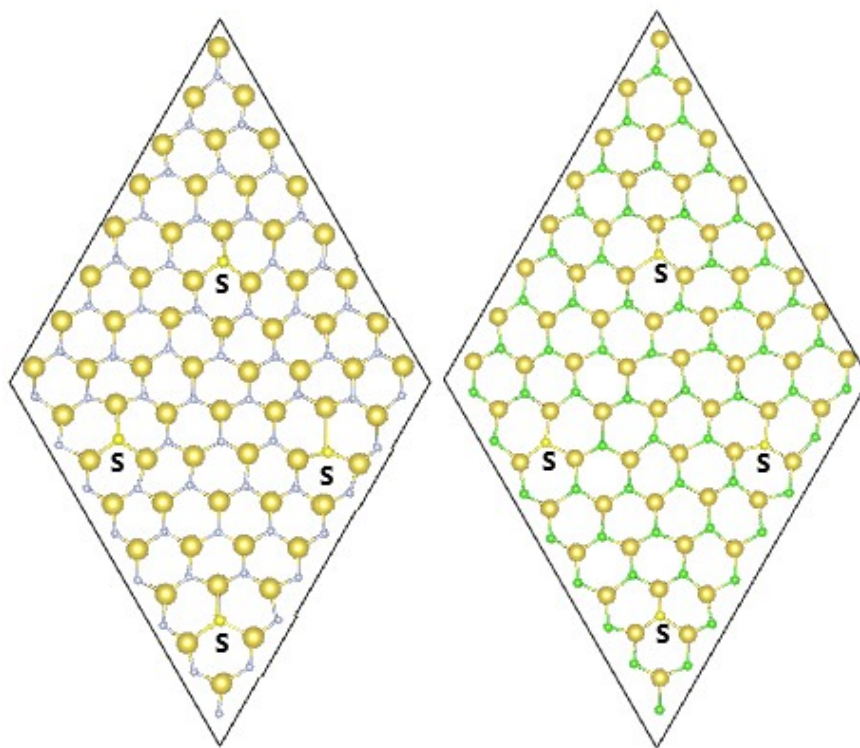


Fig.S3 (cont): Atomic structure of S-doped NaF (left side) and S-doped NaCl (right side) monolayer after 5000 fs of AIMD simulations.

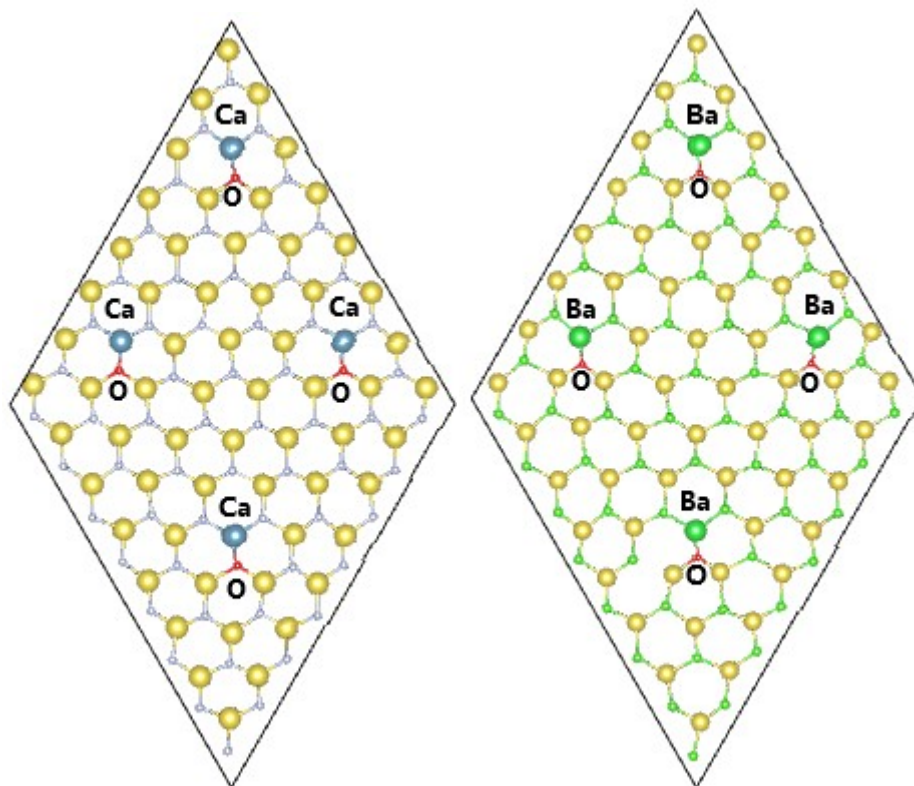


Fig.S3 (cont): Atomic structure of CaO1-codoped NaF (left side) and BaO1-codoped NaCl (right side) monolayer after 5000 fs of AIMD simulations.