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Tunable magnetic states on the zigzag edges of hydrogenated and halogenated group-IV nanoribbons FENG-CHUAN CHUANG, Natl Sun Yat-Sen Univ, TZU-CHENG WANG, Natl Taiwan Univ, CHIA-HSIU HSU, ZHI-QUAN HUANG, Natl Sun Yat-Sen Univ, WAN-SHENG SU, Natl Taiwan Sci Educ Ctr, GUANG-YU GUO, Natl Taiwan Univ — The magnetic and electronic properties of hydrogenated and halogenated group-IV zigzag nanoribbons (ZNRs) are investigated by first-principles density functional calculations. Fascinatingly, we find that all the ZNRs have magnetic edges with a rich variety of electronic and magnetic properties tunable by selecting the parent and passivating elements as well as controlling the magnetization direction and external strain. In particular, the electric property of the edge band structure can be tuned from the conducting to insulating with a band gap up to 0.7 eV, depending on the parent and passivating elements as well as the applied strain, magnetic configuration and magnetization orientation. The last controllability would allow us to develop magnetic on-off nano-switches. Furthermore, ZNRs such as SiI, Ge, GeI and SnH, have fully spin-polarized metallic edge states and thus are promising materials for spintronics. The calculated magnetocrystalline anisotropy energy can be as large as ˜9 meV/edge-site, being 2000 time greater than that of bulk Ni and Fe (˜5 μeV/atom), and thus has great potential for high density magneto-electric data-storage devices. Finally, the calculated exchange coupling strength and thus magnetic transition temperature increases as the applied strain goes from -5 % to 5 %. Our findings thus show that these ZNRs would have exciting applications in next-generation electronic and spintronic nano-devices.

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