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Abstract	Dangerous heavy metals are increasingly polluting our water, so we need better and simpler ways to clean them up. This study employs comprehensive density functional theory (DFT) simulations to meticulously investigate the structural, electronic, and adsorption properties of monolayer Gallium Sulphide (GaS) and Gallium Selenide (GaSe) quantum dots (QDs), both in their pristine and heteroatom-doped (C, N, O) forms. Novelty is introduced through the in-depth exploration of these emerging GaS and GaSe QDs as sophisticated adsorbents, moving beyond conventional materials to address the critical challenges of heavy metal removal. Our findings reveal that heteroatom doping significantly modulates the structural stability and electronic band gaps of these QDs, optimizing their reactivity. Crucially, the doped GaS/GaSe systems exhibit remarkably strong and exothermic adsorption energies towards highly toxic arsenic (As), chromium (Cr), and nickel (Ni) ions. Specifically, GaSe-Ni and GaSe-Cr systems demonstrate exceptionally strong binding, highlighting their superior immobilization capabilities. This research pioneers a detailed theoretical framework for utilizing pristine and doped GaS/GaSe QDs, providing critical insights into their interaction mechanisms with heavy metals and their potential for developing next-generation, high-performance environmental remediation.