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First-principles study on structure stabilities of α-S and Na-S battery systems[1] HIROYOSHI MOMIDA[2], TAMIO OGUCHI[3], ISIR, Osaka University — To understand microscopic mechanisms of charge and discharge reactions in Na-S batteries, there has been increasing needs to study fundamental atomic and electronic structures of elemental S as well as that of Na-S phases. The most stable form of S is known to be an orthorhombic α-S crystal at ambient temperature and pressure, and α-S consists of puckered S_8 rings which crystallize in space group *Fddd*. In this study, the crystal structure of α-S is examined by using first-principles calculations with and without the van der Waals interaction corrections of Grimme's method, and results clearly show that the van der Waals interactions between the S_8 rings have crucial roles on cohesion of α-S. We also study structure stabilities of Na_2S, NaS, NaS_2, and Na_2S_5 phases with reported crystal structures. Using calculated total energies of the crystal structure models, we estimate discharge voltages assuming discharge reactions from $2Na+xS \rightarrow Na_2S_x$, and discharge reactions in Na/S battery systems are discussed by comparing with experimental results.

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