Search for compounds that accelerate electron capture decay of ^{7}Be by first-principles calculation

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In radionuclide compounds undergoing electron capture (EC) decay, the electron density at the nucleus ($\rho(0)$) and half-life of a nucleus are inversely proportional. Using this relationship, the half-life can be tuned by changing the physical or chemical conditions. The system with the most remarkable decrease in half-life was reported in ^{7}Be contained in C_{60} fullerene. The previous study reported a reduction of approximately 1.5% in the experimental half-life of ^{7}Be contained in C_{60} compared with Be metal, and the theoretical $\rho(0)$ at the Be nucleus in C_{60} increased by approximately 1.7%.[1]

The present work theoretically investigates the mechanism of increasing $\rho(0)$ in Be compounds and identifies new systems whose half-life is lower (i.e., $\rho(0)$ is higher) compared with that of C_{60}. We performed density functional calculations with B3LYP functional by Gaussian09, and pcS-4 and 6-31G* basis sets were used for Be and other atoms, respectively. The analysis of $\rho(0)$ in some Be compounds indicates that $\rho(0)$ is generally decreased due to the electron donation from Be to other atoms through ionic, covalent, or metallic bonds. Hence, we need to seek some systems with no chemical bonds, and we focused on Be-encapsulated fullerenes of various sizes (C_{20}–C_{180}). The $\rho(0)$ of Be in C_{50} slightly increased (35.611 a.u.) compared with that in C_{60} (35.565 a.u.); however, the $\rho(0)$ in the lower-order fullerenes than C_{50} decreases because of forming chemical bonds with carbons. Hence, we focused on $\rho(0)$ in Be-encapsulated rare gas crystals (Ne, Ar, Kr) at high pressure because rare gases hardly form chemical bonds even at short distance. If a Be was encapsulated in Ar crystal at a lattice constant of 2 Å, $\rho(0)$ would increase by approximately 10% (i.e., half-life decreases by approximately 10%) compared to that of Be metal (Figure 1). The condition to form the Ar crystal at lattice constant 2 Å was estimated as 350 kbar pressure at 293K temperature based on the parameters reported in the previous study.[2] This half-life reduction is more significant than the previous work in C_{60}.

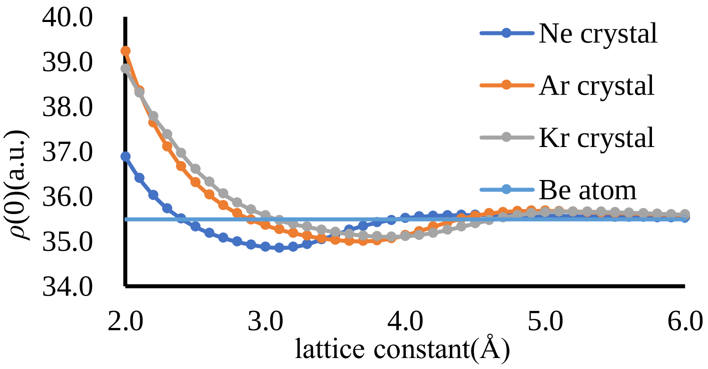

Figure 1. Relationship between lattice constants and $\rho(0)$ of Be-encapsulated rare gas crystals

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