**Theoretical study on positronium formation at metal surfaces based on two-component density functonal theory**

Satoshi Hagiwara\*, and Atsuo Kawasuso

*National Institutes for Quantum and Radiological Science and Technology,*

*1233 Watanuki, Takasaki, Gunma 370-1292, Japan.*

\* E-mail: hagiwara.satoshi@qst.go.jp

When positrons are slowly incident onto the material surfaces, a portion of the positrons diffuse back to the surface. Then, positronium (Ps), which is a bound state between an electron and a positron, is formed and spontaneously emitted into the vacuum, when its work function is negative [1]. Since normally Ps is not formed in the bulk due to the strong electron screening effect to positrons, the Ps formation spectroscopy has been expected to be a sensitive probe for the surface electronic structures. In this respect, Ps formation processes at various surfaces have been studied both theoretically [2] and experimentally [3].

Recently, an experiment using spin-dependent Ps formation and annihilation, has been carried out to investigate the surface spin-polarization of ferromagnetic surfaces covered with graphene and boron-nitride white graphene (BNWG) [4]. This study demonstrated that the Ps is formed at the first surface layer (i.e., graphene or BNWG), and the surface spin-polarization is caused by orbital hybridization between the ferromagnets and graphene or BNWG. This finding implies the potential of Ps formation spectroscopy in determining the surface electronic structure at the first atomic layer.

However, the details of the Ps formation at surface have not yet been fully understood because of the lack of theoretical study on the Ps formation using *real material surfaces.* Previous theoretical studies on the Ps formation were carried out within a jellium model or by assuming bulk electronic band structures [2]. In order to understand the Ps formation mechanism precisely, we are conducting the calculation of two-component density functional theory (TCDFT) for the Ps formation energy spectrum (PsFES) at metal surfaces. TCDFT is the one of the most flexible and powerful tool to study electronic and positronic states in real materials [5].

We found that the calculated PsFES qualitatively reproduce the experimental data. We also examined the projections of PsFES to the surface electronic band structures. Consequently, we found that the PsFES significantly depends on surface electronic states. In the presentation, we will report further details of the Ps formation processes.

1. C. Hugenschmidt, Surf. Sci. Rep. **71**, 547 (2016).
2. A. Ishii Surf. Sci. **209**, 23 (1989).
3. A. Jones et al., Phys. Rev. Lett. **117**, 216402 (2016).
4. A. Miyashita et al., Phys. Rev. B **97**, 195405 (2018).
5. M. Puska and R. Nieminen Rev. Mod. Phys. **66**, 841 (1994).