

## Spin-related bands in surface-enhanced Raman scattering spectra for classification of rare earth ions

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Surface-enhanced Raman scattering (SERS) spectra of different rare earth (RE) ion-citrate complexes were investigated for the first time for RE ion classification. With the addition of rare earth ions into silver nanoparticles in aqueous solution, the Raman signals of RE-citrate complexes were significantly enhanced and the characteristic peaks near  $1070\text{ cm}^{-1}$  and  $1315\text{ cm}^{-1}$  were appeared. The relative intensities of these peaks did not change with changing the laser wavelengths of 488 nm and 532 nm. RE-citrate complexes including RE ions effects were analyzed based on density functional theory (DFT) calculations. Calculation results show that these characteristic peaks are related to the carboxyl and hydroxyl coordination of RE ions and citrate (Figure 1(a) and (b)), indicating these are spin-related bands of RE ions. Thus, different RE ions were classified by a ratio of characteristic SERS peaks near  $1070\text{ cm}^{-1}$  and  $1315\text{ cm}^{-1}$ (Figure 1(c)-(e)). Further discussion will be shown in the poster presentation.

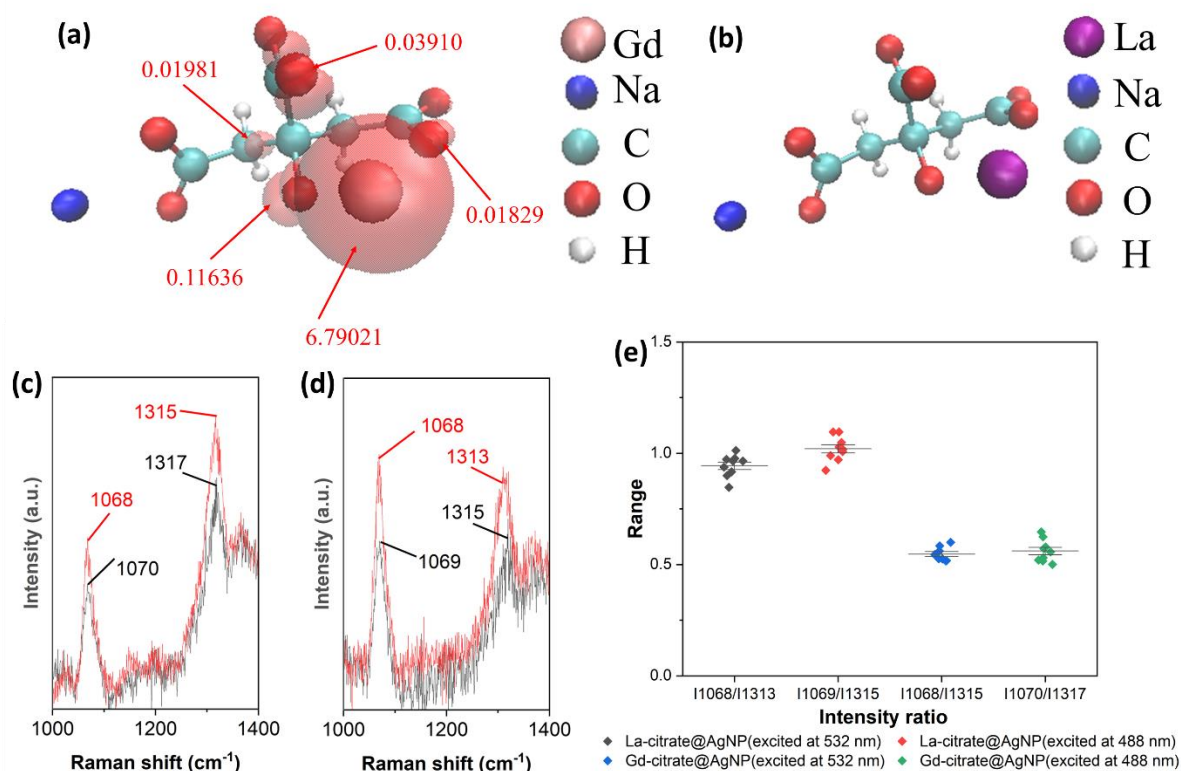


Figure 1. (a) and (b): Structure and spin population of (a) Gd-citrate and (b) La-citrate complexes. (c) and (d): Characteristic peaks at around  $1070\text{ cm}^{-1}$  and  $1315\text{ cm}^{-1}$  in SERS spectra of (c) Gd-citrate and (d) La-citrate. (e): Ratios of intensities of characteristic peaks under different excitation laser wavelength for ion classification of Gd and La.