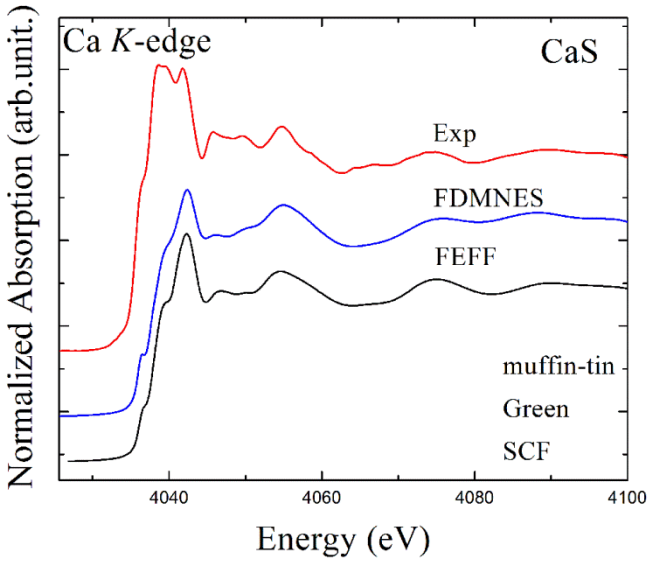
Electronic supplementary materials

Electronic structure and hybridization of CaS by means of X-ray absorption spectroscopy at Ca and S *K*-edges

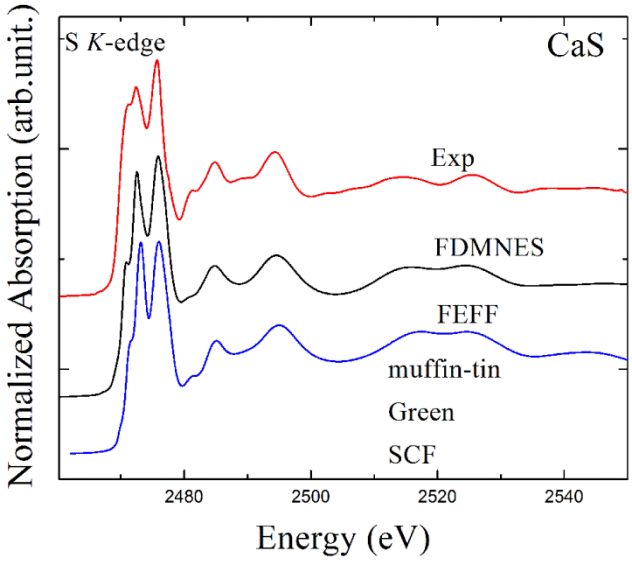
Wei Xu[a]*, Lijuan Liu[a], Mingqi Cui[a], Lei Zheng[a], Yongfeng Hu[b], Augusto Marcelli[ac] and Ziyu Wu[d]*

[a]Insitute of High Energy Physics, Chinese Academy of Sciences, Beijing, 100049, People's Republic of China, [b]Canadian Light Source, University of Saskatchewan, Saskatoon, Canada, [c]Laboratori Nazionali di Frascati, Istituto Nazionale di Fisica Nucleare, Frascati, Rome, 00044, People's Republic of China, and [d]National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, 230026, People's Republic of China

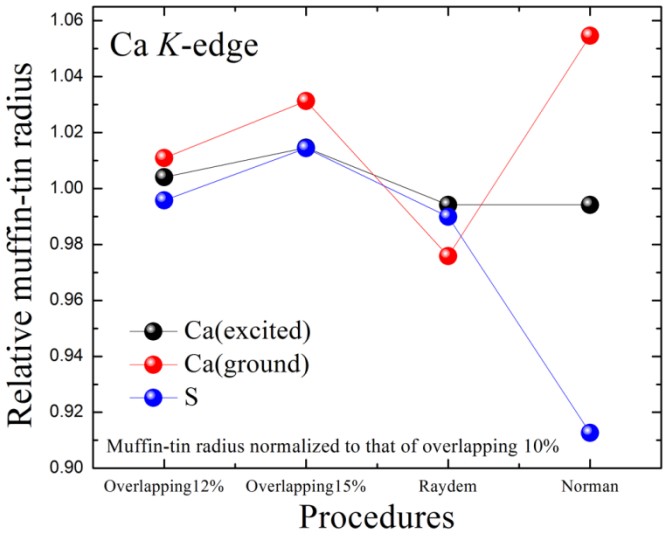
Correspondence email: xuw@mail.ihep.ac.cn; wuzy@ustc.edu.cn



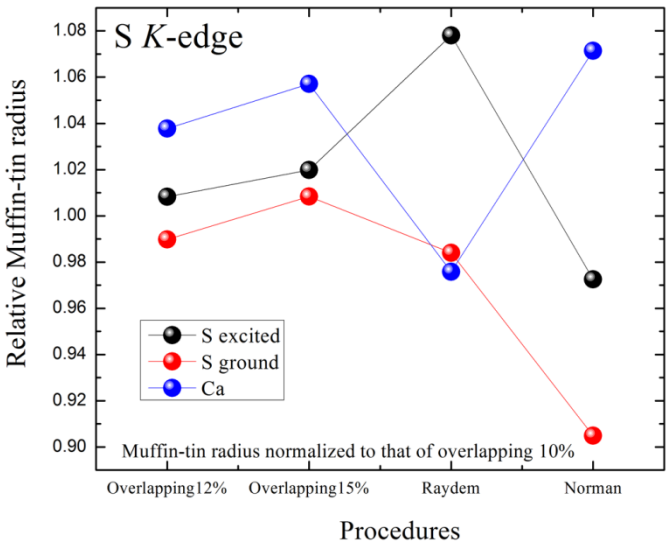
FigureS1. Comparison of Ca *K*-edge experimental and theoretical XANES spectra calculated using Green function and SCF potential procedure in the framework of Multiple Scattering Theory with muffin-tin potentials, as implemented by FDMNES and FEFF9.0 code, respectively. The atomic cluster with radius of 12Å is selected for both simulations.



FigureS2. Comparison of S *K*-edge experimental and theoretical XANES spectra calculated using Green function and SCF potential procedure in the framework of Multiple Scattering Theory with muffin-tin potentials, as implemented by FDMNES and FEFF9.0 code, respectively. The atomic cluster with radius of 12Å is selected for both simulations.



FigureS3. The evolvement of muffin-tin radii for different atoms in different procedures as simulating the Ca *K*-edge XANES; all muffin-tin radii are normalized to the muffin-tin radius of overlapping 10%.



FigureS4. The evolvement of muffin-tin radii for different atoms in different procedures as simulating the S *K*-edge XANES; all muffin-tin radii are normalized to the muffin-tin radius of overlapping 10%.

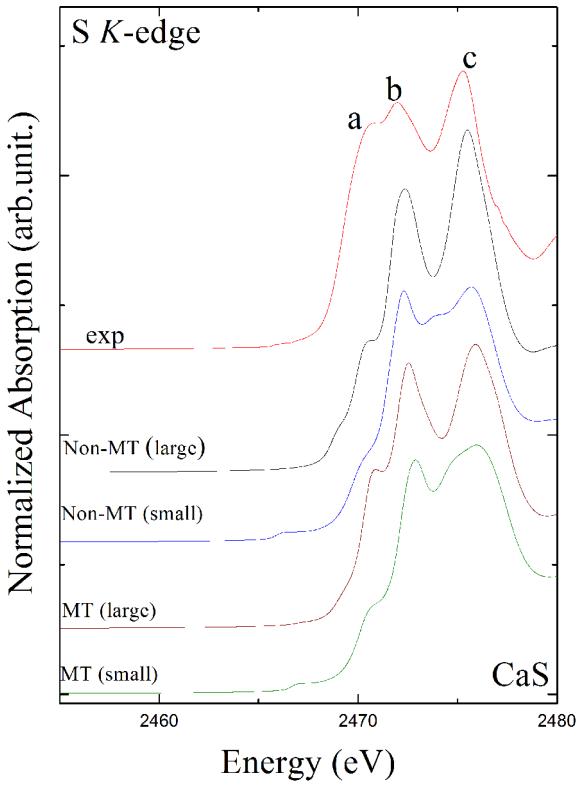


Figure.S5 Pre-edge feature at S *K*-edge

As shown in Figure.S5 For sulfur *K*-edge, the pre-edge "foot" is not shown in experimental spectrum. It is only present in the theoretical spectra calculated using small cluster. The difference is due to the Fermi level determined from different sizes of clusters. The Fermi level is more reliable for large clusters. In other words, only the large cluster produces better results. In Table S1, we listed the Fermi energy for comparison.

Table S1. The Fermi level determined from different cluster size for MT and non-MT methods.

	Cluster for potential	Fermi level(eV)
Non_MT_large	14.50(587 atoms)	-5.06348
MT_large	14.50(587 atoms)	-5.06348
Non_MT_Small	9.50(171atoms)	-5.27664
MT_Small	10.50(203 atoms)	-5.38103

Back to the question, the system is quite unique that the Fermi energy can be accurately determined with extremely large clusters.