Geodynamics Seminar

第352回ジオダイナミクスセミナー

Ab initio computation on the Fe L-edge X-ray emission spectroscopy of Fe-bearing MgSiO3 perovskite

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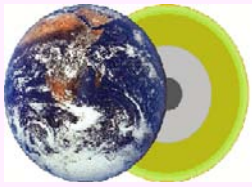
主催：愛媛大学地球深部ダイナミクス研究センター
日時：3/8（金）午後 4時30分～
場所：総合研究棟 4F 会議室



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Abstract

Since the L-edge X-ray emission spectroscopy (XES), a 3d to 2p transition, can directly illustrate features of 3d electrons, to identify Fe's behaviors in MgSiO3 perovskite (Pv) under the lower mantle conditions, the L-edge XES of Fe2+- and Fe3+-bearing Pv under high pressure were simulated based on the internally consistent LSDA+U technique combined with the Slater-transition method. The spin transition, from the high spin state to the low spin state, of Fe2+ and Fe3+ can be identified easily by detecting shifts of main peaks across the spin transition. The valence state of Fe (2+ or 3+) can be furthermore certified similarly, since the shift of the first main peak of Fe2+across the spin transition of 2 eV, in good agreement with the experimental value (~1.6 eV), is significantly smaller than that of Fe3+ of 4 eV. The width of the L-edge XES of Fe3+ also depends strongly on the substitūtion sites (Mg or Si site), meaning that coordination environments Fe might also be distinguishable based on the Fe L-edge XES spectra. These strong sensitivities to the Fe states suggest that the high-resolution Fe L-edge XES measurement would be a useful experimental technique to investigate Fe-bearing silicate minerals.

詳細は当センターホームページ: http://www.ehime-u.ac.jp/~grc/をご覧ください
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