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Charge carriers in spinel AlV_2O_4 order below 700K

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AlV_2O_4 with the spinel structure shows some magnetic and electric anomalies around 700K, which originate from the formation of the charge ordered (CO) structure.[1,2] In this talk, we will report a structural model of the CO structure in AlV_2O_4 , which was obtained by electron diffraction, synchrotron x-ray diffraction and magnetic measurements. The CO structure is characterized by the formation of V clusters “heptamers”, each of which is consisting of 7 vanadium atoms and is in a spin- singlet state as a total. Note that the number of electrons per site is still fractional in this CO structure. In addition, theoretical consideration suggests that this unique molecular-like V heptamer is stabilized by a strong bonding of vanadium t_{2g} orbitals. This work has been done in collaboration with Drs. S. Mori, T. Katsufuji, Y. Motome, N. Furukawa, H. Ishibashi, N. Ikeda and K. Kato. [1]K. Matsuno,et al., J. Phys. Soc. Jpn. **70**, 1456 (2001). [2]K. Matsuno et al., Phys. Rev. Lett. **90**, 096404 (2003).