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Separation of a molecular electronic configuration transition from the spin-crossover transition XIN ZHANG, SAI MU, University of Nebraska-Lincoln, JIA CHEN, Columbia University, GUILLAUME CHASTANET, DARO NATHALIE, JEAN-FRANÇOIS LÉTARD, TATIANA PALAMARCIUC, PATRICK ROSA, Université de Bordeaux, JING LIU, DARIO ARENA, GEORGE STERBINSKY, Brookhaven National Laboratory, BOHDAN KUNDYS, BERNARD DOUDIN, Université Louis Pasteur Strasbourg, PETER A. DOWBEN, University of Nebraska-Lincoln — We have investigated the unoccupied electronic structure of several molecular spin crossover systems including [Fe(H_2B(pz)$_2$)$_2$(bipy)] [Fe(H_2B(pz)$_2$)$_2$phen], [Fe(PM-AzA)$_2$(NCS)$_2$] and [Fe(phen)$_2$(NCS)$_2$] by inverse photoemission (IPES) and X-ray absorption spectroscopy (XAS). The XAS clearly shows the change of iron L2 edge spectra, typically associated with thermal induced spin crossover, occurring at temperatures well below the temperatures of the spin crossover transition. This suggests a change in the electronic structure configuration occurring separately from the spin ordering from a low spin to high spin state. These results may be significant to understand the observations that indicate that the spin crossover transition, and certainly the unoccupied electronic structure, is influenced by electric field. In some respects, these results for the molecular spin crossover transition resemble the separation of the charge ordering transition from the ferromagnetic transition in the manganates.

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