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Changes in the unoccupied electronic structure of [Fe($H_2B(pz)_2)_2$(bipy)] thin films YANG LIU, XIN ZHANG, SUMIT BENIWAL, AXEL ENDERS, Univ of Nebraska - Lincoln, PATRICK ROSA, JEAN-FRANÇOIS LÉTARD, TATIANA PALAMARCIUC, Université de Bordeaux, JING LIU, DARIO ARENA, National Synchrotron Light Source, BERNARD DOUDIN, Université Louis Pasteur Strasbourg, PETER A. DOWBEN, Univ of Nebraska - Lincoln, GROUPE DES SCIENCES MOLÉCULAIRES, UNIVERSITÉ DE BORDEAUX COLLABORATION, BROOKHAVEN NATIONAL LABORATORY, NATIONAL SYNCHROTRON LIGHT SOURCE COLLABORATION, INSTITUTE DE PHYSIQUE APPLIQUE DE PHYSIQUE ET CHIMIE DES MATERIAUX DE STRASBOURG, UNIVERSITÉ LOUI COLLABORATION — We have investigated the unoccupied electronic structure of ultra thin films of the spin crossover [Fe($H_2B(pz)_2)_2$(bipy)] complex (with $H_2B(pz)_2$ =bis(hydrido)bis(1H-pyrazol-1-yl)borate and bipy = 2,2'-bipyridine) deposited on Au(111) by inverse photoemission (IPES) and X-ray absorption spectroscopy (XAS). The XAS clearly shows the changes of iron L edge spectra typically associated with thermal induced spin crossover and found to be very consistent with the changed of the lowest unoccupied molecular orbitals seen in inverse photoemission with temperature. A band gap of 2-3 eV is deduced from combined UPS and IPES measurements of the films on Au substrates. The shift of the unoccupied density of states seen in inverse photoemission and XAS, with temperature, differs little from the molecular powder suggesting little influence of the substrate. We suggested that the ordering of this spin-crossover molecule on the gold substrate, may lead to a small anisotropy energy, for the molecular high spin state.

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