



## FLASH INFO N°15 – AVRIL 2024

### Spécial webinaire

Dear Colleague,

The Electron Spectroscopy Division of the French Vacuum Society cordially invites you to participate to the 7<sup>th</sup> edition of its scientific webinars, to be held Wednesday, April 3rd, 2024 at 4:00 pm, on the topic below :

45 min, including questions)

*"Does inverse photoemission have sufficient value to outweigh the difficulties ?"*

Presented by:

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Abstract:

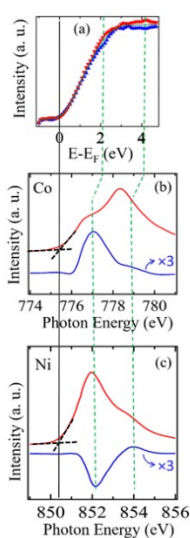
With the availability of commercial inverse photoemission systems, inverse photoemission may become more widely available, but count rates and resolution are remain low compared to photoemission. Yet it is worth noting that inverse photoemission, in combination with other techniques, can provide valuable insights. Angle resolved inverse photoemission can be used to experimentally map out the conduction (unoccupied) band structure in much the same way as angle-resolved photoemission is widely used to map out the valence (occupied) band structure. The combination of angle-resolved photoemission and angle resolved inverse photoemission provides several insights that theory presently cannot. From this combination of angle-resolved photoemission and angle resolved inverse photoemission, we find examples where density functional theory has good agreement with experiment for the occupied states (the valence band) but agreement for the unoccupied states (conduction band) is less reliable [1]. This combination of techniques also allows one to determine the effect of conducting substrates on the highest occupied molecular orbital (HOMO) to lowest unoccupied molecular orbital (LUMO) gap of a molecular adsorbate [2-4], molecular band offsets [5-9] and molecular band realignment with doping [10], all of which are key device parameters in molecular electronics not easily extracted from theory. Combining spin-polarized inverse photoemission with X-ray magnetic circular dichroism allows one to assign the spin polarized unoccupied bands to transition metal spectra weights in multi-elemental magnetic materials [11,12]. As is widely recognized, the surface is not the bulk of a material and inverse photoemission is highly surface sensitive, more so than photoemission, thus not suitable for characterizing the bulk electronic structure. One can speculate that inverse photoemission is not going to be very appealing to many in the materials science community in part because it is so highly surface sensitive (so the surface has to be well characterized), and count rates are low. Inverse photoemission is also wave-vector dependent and so spin-polarized inverse photoemission is not a better measure of the true surface polarization than spin-polarized photoemission and can only be considered an indicator. Just the same I hope here to demonstrate inverse photoemission does have value.

- [1] T. Komesu, D. Le, Xin Zhang, Q. Ma, E. F. Schwier, Y. Kojima, M. Zheng, H. Iwasawa, K. Shimada, M. Taniguchi, L. Bartels, T. S. Rahman and P. A. Dowben, Applied Physics Letters 105 (2014) 241602;
- [2] J. Zhang, D.N. McIlroy, P.A. Dowben, H. Zeng, G. Vidali, D. Heskett and M. Onellion, J. Phys. Cond. Matt. 7 (1995) 7185-7194
- [3] D.N. McIlroy, J. Zhang, P.A. Dowben and D. Heskett, Mat. Sci. Eng. A 217/218 (1996) 64-68
- [4] Jie Xiao and Peter A. Dowben, J. Materials Chem. 19 (2009) 2172-2178
- [5] J. Liu, J. Xiao, S.-B. Choi, P. Jeppson, L. Jarabek, Ya.B. Losovyj, A.N. Caruso and P.A. Dowben, J. Physical Chemistry B 110 (2006) 26180-26184
- [6] Jie Xiao, Andrei Sokolov, P.A. Dowben, Appl. Phys. Lett. 90 (2007) 242907
- [7] Jie Xiao and P.A. Dowben, J. Phys. Cond. Matter 21 (2009) 052001
- [8] P. E. Evans, T. Komesu, E. F. Schwier, S. Kumar, K. Shimada, P. A. Dowben, J. Physics: Condensed Matter 32 (2020) 465001
- [9] T. Komesu, D. Le, Iori Tanabe, E. F. Schwier, Y. Kojima, M. Zheng, K. Taguchi, K. Miyamoto, T. Okuda, H. Iwasawa, K. Shimada, T. S. Rahman and Peter A. Dowben, J. Phys. Cond. Matter 29 (2017) 285501
- [10] P.A. Dowben, Jie Xiao, Bo Xu, Andrei Sokolov, and B. Doudin, "Different Approaches to Adjusting Band Offsets at Intermolecular Interfaces", Appl. Surf. Sci. 254 (2008) 4238-4244
- [11] C. N. Borca, Takashi Komesu, Hae-Kyung Jeong, P.A. Dowben, Delia Ristoiu, Ch. Hordequin, J. P. Nozières, and J. Pierre, Shane Stadler and Y. U. Idzerda, Physical Review B 64 (2001) 052409
- [12] C. Mellinger, X. Wang, A. Subedi, A. T. Clark, T. Komesu, R. Rosenberg, P. A. Dowben, X. Cheng, X. Xu, J. Appl. Phys. 133 (2023) 195301



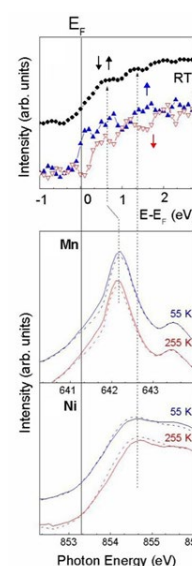
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On the left, the comparison of the spin-polarized inverse photoemission (a), X-ray circular dichroism (b and c, blue spectra), and X-ray absorption spectra for NiCo<sub>2</sub>O<sub>4</sub> thin films (red spectra, b and c). The XMCD spectra have been magnified by three times for better visualization. From: C. Mellinger, et al., J. Appl. Phys. 133 (2023) 19530.

On the right, the comparison of the spin-polarized inverse photoemission (top) and X-ray absorption spectra spectra for NiMnSb(100). From: C. N. Borca, Takashi Komesu, Hae-Kyung Jeong, P.A. Dowben, Delia Ristoiu, Ch. Hordequin, J. P. Nozières, and J. Pierre, Shane Stadler and Y. U. Idzerda, Physical Review B 64 (2001) 052409. The black vertical line aligns the Fermi level, and the dashed lines indicate the possible correspondence between unoccupied states in X-ray absorption/X-ray circular dichroism spectra.



*Pour vous abonner au Flash Info trimestriel de la Division, renseignez le formulaire «Besoin d'info?» sur le portail du Comité Spectroscopie d'Electrons. Retrouvez-y également d'autres informations utiles : conférences, nouveaux périodiques, publications... !*