



Colloquium Announcement

of the Collaborative Research Centre 951

“Hybrid Inorganic/Organic Systems for Opto-Electronics”

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Optoelectronic Devices based on Two-dimensional Materials for Neuromorphic Edge Applications

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Ab initio electron dynamics at hybrid interfaces: Lessons learned

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Optoelectronic Devices based on Two-dimensional Materials for Neuromorphic Edge Applications

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My group is developing a new paradigm of sensing, computing, storage, and hardware security inspired by the neurobiological architectures and neural algorithms found inside various animal brains that allow evolutionary success in resource constrained environments. Towards the realization of our vision, we exploit unique electronic and optoelectronic properties of layered two dimensional (2D) materials such as graphene, MoS₂, WSe₂, black phosphorous etc., to design high performance, ultra-low-power, artificially intelligent, and inherently secure solid state devices inspired by natural intelligence. For example, we have mimicked auditory information processing in barn owl ([Nature Communications, 10, 3450, 2019](#)), collision avoidance by locust ([Nature Electronics, 3, 646–655, 2020](#)), and subthreshold signal detection by paddlefish and cricket using stochastic resonance ([Nature Communications, 2020](#)). We have also mimicked probabilistic computing in animal brains using low-power Gaussian synapses ([Nature Communications, 10, 4199, 2019](#)), and memristive graphene synapses ([Nature Communications, 11, 5474, 2020](#)) and realized biomimetic devices that can emulate neurotransmitter release in chemical synapses ([ACS Nano, 11, 3, 2017](#)) and neural encoding in afferent neurons ([Nature Communications, 12, 2143, 2021](#)). We have also made these device secure through SAT-attack resistant hardware obfuscation using camouflaged 2D heterostructures ([ACS Nano, 15, 2, 2021](#)) and by realizing machine learning resilient and reconfigurable physically unclonable functions ([Nature Electronics 4, 364-374, 2021](#)).

***Ab initio* electron dynamics at hybrid interfaces: Lessons learned**

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The peculiar electronic structure of inorganic/organic interfaces formed by low-dimensional semiconductors and carbon-conjugated molecules gives rise to unique light-matter coupling phenomena. The interaction with time-dependent electric fields of femtosecond duration offers the opportunity to disclose the birth of excitations and to monitor the key mechanisms ruling charge-transfer and its dynamics in these materials. Adopting real-time time-dependent density functional theory in conjunction with Ehrenfest molecular dynamics, we have been investigating these phenomena from first principles. In this colloquium, I will show the highlights of this research focusing in particular on the role played by the intensity of the external field [1], by the coupling between electronic and vibrational degrees of freedom [2], as well as by the dielectric characteristics of the surrounding [3]. In addition, I will share some important lessons that we learned along this journey, both from a methodological standpoint [4] as well as regarding the fundamental properties of the considered hybrid interfaces [5-7].

References:

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- [3] C. Cocchi, M. Guerrini, J. Krumland, N. T. Nguyen, and A.M. Valencia, *J. Phys.: Materials* 6, 012001 (2022).
- [4] J. Krumland, M. Jacobs, and C. Cocchi, *PRB* 106, 144304 (2022).
- [5] J. Krumland and C. Cocchi, *Electron. Struct.* 3, 044003 (2021).
- [6] G. Melani, J. P. Guerrero-Felipe, A. M. Valencia, J. Krumland, C. Cocchi, and M. Iannuzzi, *PCCP* 24, 16671 (2022).
- [7] H. Hamdi, J. Krumland, A. M. Valencia, C-A. Palma, and C. Cocchi, *in preparation*.