Tautology, Oxymoron, or a matter of timescales? Defects and Halide Perovskites

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Results of optical and electrical measurements show low to ultra-low of optoelectronically active defect densities in materials, prepared near STP from organic solvents. The two leading rationalizations for these low defect densities are Self-Healing, SH, and Defect Tolerance, DT. Using simple *logic arguments,* it was shown that even DT must include an active reaction to damage[2], such as SH, which was invoked also to explain the behavior of $CuInSe_2$ (→CIGS)[1]. For 3D HaPs experimental evidence has been presented for SH, a process that, in inanimate matter, is explained by equilibrium thermodynamics.[3] To this body of data are now added recovery from photodamage results on 2D and 2D-3D HaP *single crystals*, which can be compared to results on 3D ones.[4] Such healing and the resulting low defect density can be rationalized thermodynamically and kinetically by the small ΔG and activation energy for formation (and decomposition). on the atomic level it is likely connected to the lattice dynamics and, as such the mechanism appears different from other repair and healing types.[2,5] To follow the arguments and models it is important to distinguish between static defects, of the textbook kind, familiar also for semiconductors, and dynamic ones, which is where time scales enter and my hope for a constructive Quantsol discussion on the issue.

* Work done with D R Ceratti, S Elboher-Aharon, G Hodes, L Kronik, S Kumar, I Lubomirsky, Y Rakita & others.

[1] Guillemoles et al., *Adv. Mat*. (1999); [2] Cahen, Hodes, Kronik, *ACS En.Lett.* (2021); [3] Ceratti et al., *Mat. Hor*.(2021); *Adv. Mat*. (2018); [4] Aharon et al.,submitted; [5] Rakita et al., *Mater. Hor*. (2019); Kumar et al., *MRS Bull.*(2020).