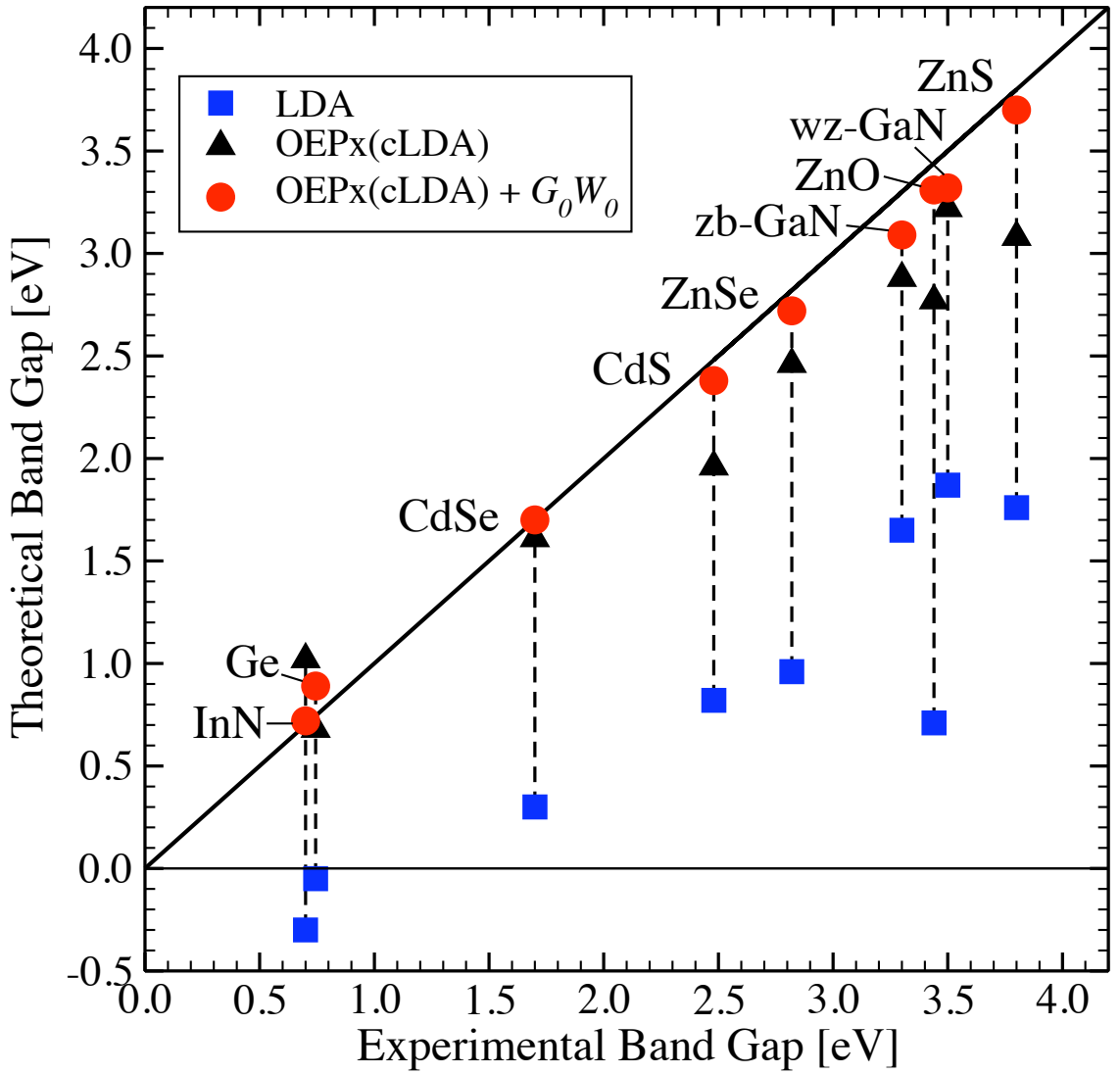
Band Gaps – OEPx and G_0W_0@OEPx



Rinke *et al. New J. Phys.* **7**, 126 (2005), phys. stat. sol. (b) **245**, 929 (2008)

How to make pseudopotential-*GW* work

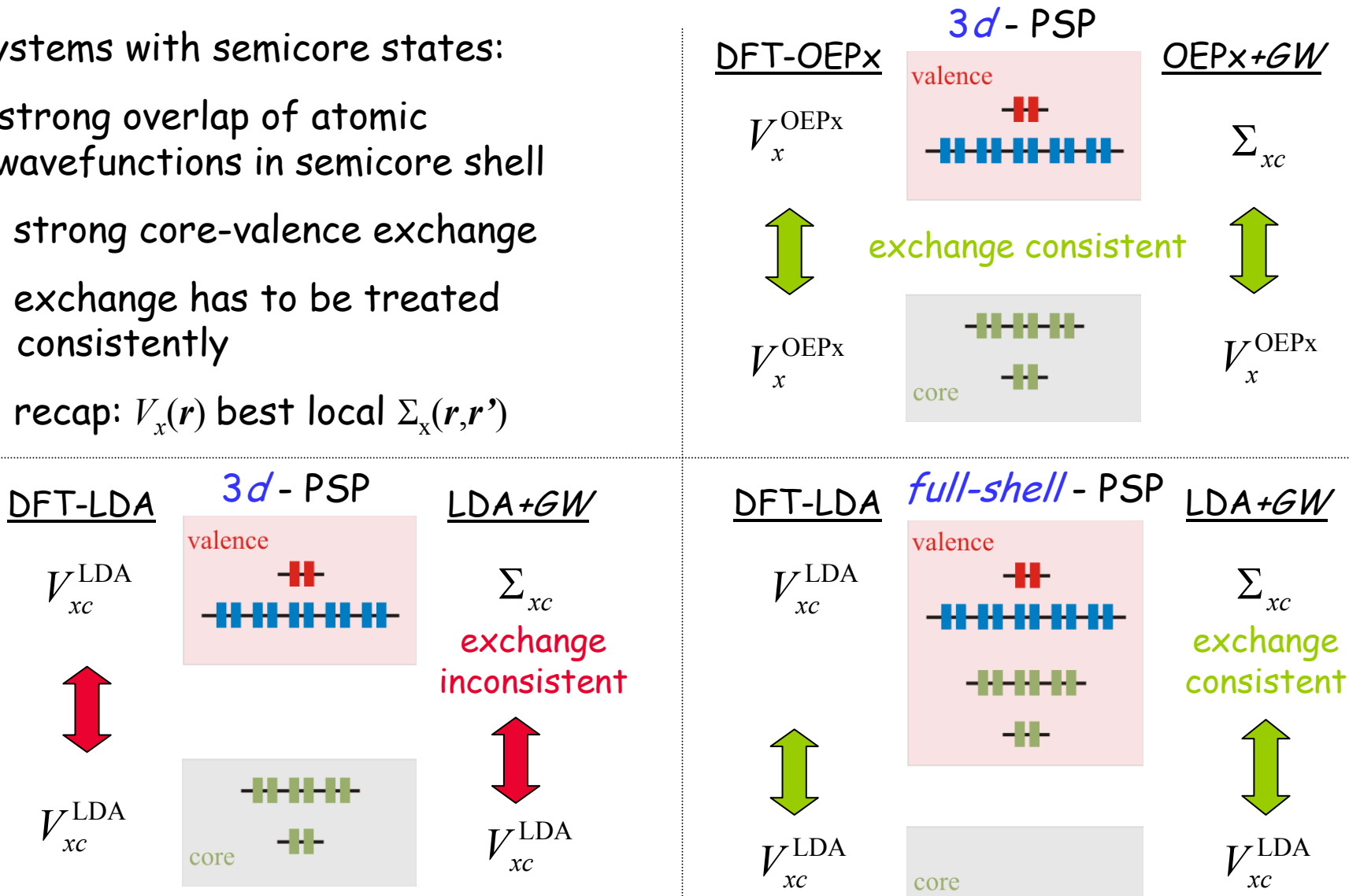
systems with semicore states:

- strong overlap of atomic wavefunctions in semicore shell

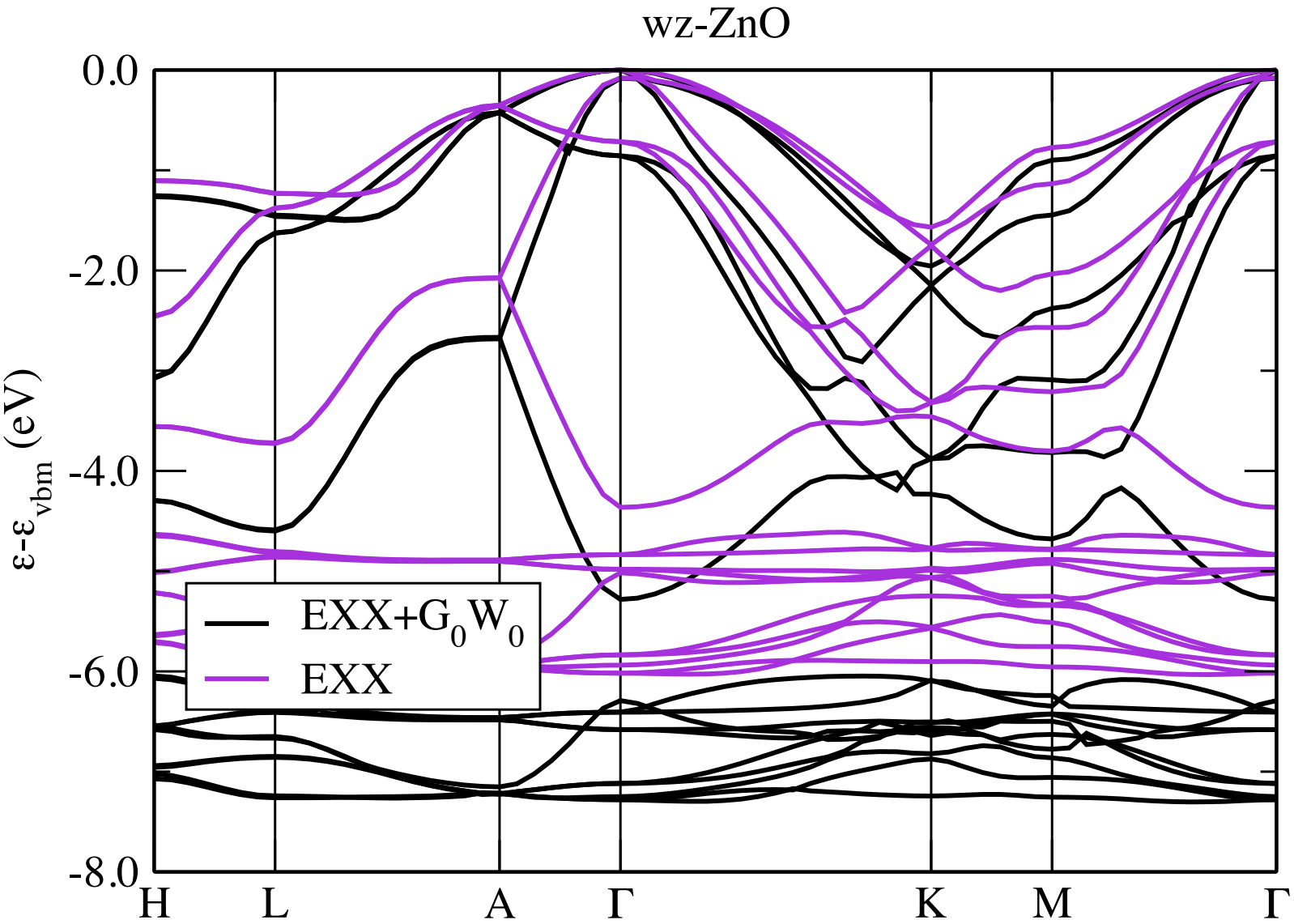
⇒ strong core-valence exchange

⇒ exchange has to be treated consistently

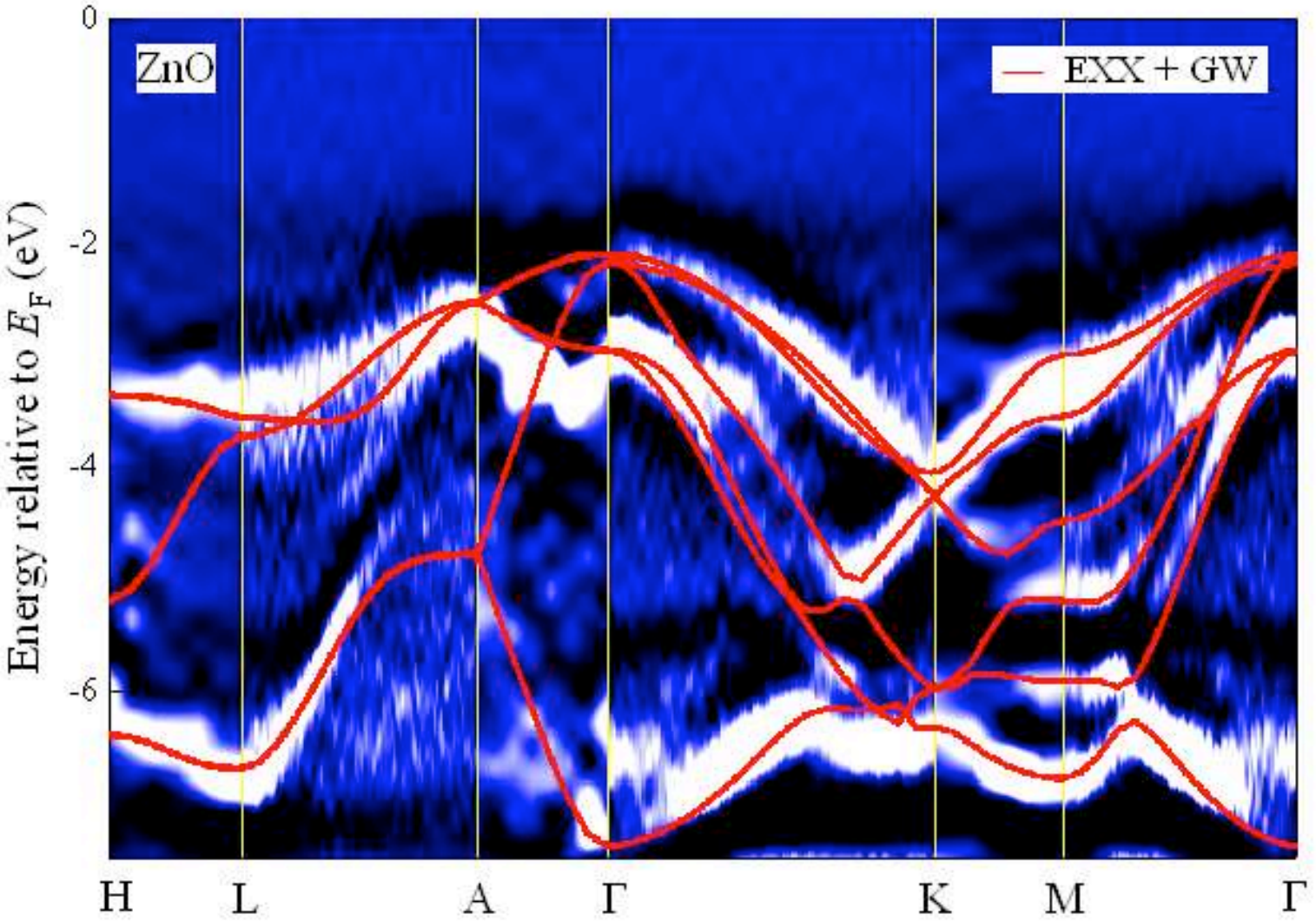
⇒ recap: $V_x(r)$ best local $\Sigma_x(r,r')$



OEPx *vs* *GW*: wurtzite ZnO



ARPES – *GW*: wurtzite ZnO



ARPES data courtesy of Masaki Kobayashi, PhD dissertation