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Van der Waals Interactions: Beyond Energies ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der MPG — The strong and ubiquitous influence of van der Waals (vdW) interactions on the structure and stability of molecules and materials is well established by now. However, much less is known about the role of vdW interactions in electronic and response properties of molecules, solids, and interfaces between them. We have recently developed and coded a fully self-consistent implementation of the Tkatchenko-Scheffler vdW density functional, enabling us to categorically assess the role of long-range vdW interactions beyond trivial energetic stabilization. We demonstrate that vdW interactions have a significant impact (and improve agreement with experiment) for HOMO-LUMO gaps, dipole moments, and polarizabilities of "chemically bound" alkali dimers. We rationalize this result based on Feynman's view on vdW interactions arising from electrostatic-like picture [1] rather than from the more conventional electrodynamic model. Finally, the role of vdW interactions on workfunctions and charge transfer in hybrid organic/metal interfaces, as well as elastic properties of molecular materials will be shortly discussed. [1] R. P. Feynman, Phys. Rev. 56, 340 (1939).

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