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A New Approach for Surface Energy Calculations Applicable to High-throughput Design of New Interfaces[1] CHRISTIAN RATSCH, JAKUB KAMINSKI, UCLA — In this talk we will present a new approach for the calculation of surface energies of periodic crystal. For non-polar materials slabs (which are terminated by two identical surfaces) the task of calculating the surface energy is trivial. But it is more problematic for polar systems where both terminating surfaces are different, as there is no single established method allowing for equal treatment of a wide range of surface morphologies and orientations. Our proposed new approach addresses this problem. It relies on carefully chosen capping atoms and the assumptions that their bond energy contributions can be used to approximate the total energy of the surface. The choice of the capping atoms is governed by a set of simple guidelines that are applicable for surfaces with different terminations. We present the results for different semiconductor materials and show that our approach leads to surfaces energies with errors as low as 2%. We show that hydrogen is not always the best choice for a capping atom if accurate surface energies are the target of the calculations. Our approach is suitable for high-throughput screening of new material interfaces, as accurate calculations of surface energies can be performed in an unsupervised algorithm.

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Christian Ratsch
UCLA

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