

PREFACE

Stepped surfaces

To cite this article: Ludo Juurlink 2018 *J. Phys.: Condens. Matter* **30** 090301

View the [article online](#) for updates and enhancements.



IOP | ebooks™

Bringing you innovative digital publishing with leading voices to create your essential collection of books in STEM research.

Start exploring the collection - download the first chapter of every title for free.



Preface

Stepped surfaces

Ludo Juurlink

Leiden Institute of Chemistry,
Leiden University, PO
Box 9502, 2300 RA Leiden,
Netherlands

E-mail: l.juurlink@chem.leidenuniv.nl

The explanation of spot splitting in low energy electron diffraction (LEED) patterns of surfaces vicinal to low Miller-index planes by Ellis and Schwobbel [1] and Henzler [2] opened the doors to studying how atomic steps influence adsorption of atoms and molecules. The earliest papers discussing such topics for macroscopically flat, but microscopically highly corrugated surfaces, thus stem from the early 1970s, adsorption and reaction initially being studied by LEED [3], flash desorption [4] and molecular beam techniques [5]. This special issue on *Adsorption Phenomena on Stepped Surfaces* starts with a historical perspective by Woodruff from Warwick University [6]—one of the first scientists who also explored the use of curved single crystals to probe the effects of steps on adsorption and reaction [7].

One of the most widely accepted ideas resulting from several decades of research on stepped surfaces is that the low-coordinated atoms in the step have an increased ability to dissociate adsorbing molecules. The origin of this effect is generally explained by an increased binding energy of the fragments as compared to the low Miller plane. Nørskov *et al* showed 15 years ago that scaling relations between the adsorption energy of dissociated diatomics and the activation barrier for dissociative adsorption also hold on stepped surfaces [8]. Defect sites on catalytic particles, which strongly resemble steps on single crystals, turn out to be crucial to various industrial catalytic processes [9, 10]. They may also be important to processes that ultimately change the selvege or bulk of the material, e.g. in bulk oxidation or metal-hydride formation. This special issue includes a paper by Farber *et al* that investigates to what extent step defects induce absorption of O atoms into the selvedge of Pt [11].

The energetics of molecular adsorption does, on the other hand, not always differ much for adsorption to steps and terraces. An example is provided in this issue in a combined density functional theory (DFT) and temperature programmed desorption study for CO adsorbing to Cu surfaces with (1 0 0) planes by Kokalj *et al* [12]. Recently, a similar combined experimental and theoretical reaction dynamics study also showed that steps can even lower reactivity—Cu(2 1 1) was shown to be less reactive toward hydrogen dissociation than Cu(1 1 1) [13].

The adsorption of larger molecules on steps has also attracted considerable interest. For tri-atomics, H₂O stands out as the binding and reaction of water with corrugated metal interfaces is highly relevant to, e.g. electrochemistry [14]. Steps influence the adsorption of water, often by inducing adsorption structures deviating rather drastically from the molecular ordering in bulk hexagonal ice, *I_h*. Steps can induce one-dimensional chain formation along edges with uncommon structural features on Pt [15], 2D patterning that includes pentamers, hexamers and octamers on Cu [16] and have even been shown to be the origin of growth of uncommon 3D cubic ice, *I_C* [17].

This special issue on *Adsorption Phenomena on Stepped Surfaces* provides two examples of studies investigating much larger molecules. Gellman *et al* use the inherent chirality of kinked-stepped surfaces and beautifully show how small variations in the interaction with a chiral cyclohexanone-derivative depends on more than chirality alone [18]. Jiang *et al* investigate the influence of benzene adsorption on work function changes [19], showing how theoretical treatment is progressing by including van der Waals interactions in their DFT study and using a range of Ag stepped surfaces extending up to seven atom-wide terraces.

The contributions in the issue show that, whereas nearly five decades of research has taught us much on how steps alter the properties of surfaces, there is still much to learn and discover. For that reason the recent revival of the use of curved samples is of high interest. With similar sizes as regular flat samples, the curved ones provide step density variations that may span up to three orders of magnitude while remaining suitable for study in many

laboratories. They have recently proven their use in studies of physical aspects, e.g. mapping of surface electronic state dependencies on stepped surface structure [20], and chemical aspects, e.g. adsorption and desorption of CO [21, 22] and H₂O [23], and chemical reactivity for elementary dissociative reactions [24] and overall reactivity [25].

ORCID iDs

Ludo Juurlink  <https://orcid.org/0000-0002-5373-9859>

References

- [1] Ellis W P and Schwoebel R L 1968 *Surf. Sci.* **11** 82–98
- [2] Henzler M 1970 *Surf. Sci.* **19** 159–71
- [3] Lang B *et al* 1972 *Surf. Sci.* **30** 454–74
- [4] Lu K E and Rye R R 1974 *Surf. Sci.* **45** 677–95
- [5] Bernasek S L and Somorjai G A 1975 *J. Chem. Phys.* **62** 3149–61
- [6] Woodruff D P 2016 *J. Phys.: Condens. Matter* **28** 491001
- [7] Armitage A F *et al* 1980 *Surf. Sci.* **100** L483–90
- [8] Nørksov J K *et al* 2002 *J. Catal.* **209** 275–8
- [9] Honkala K *et al* 2005 *Science* **307** 555–8
- [10] Behrens M *et al* 2012 *Science* **336** 893–7
- [11] Farber R G *et al* 2017 *J. Phys.: Condens. Matter* **29** 164002
- [12] Kokalj A *et al* 2017 *J. Phys.: Condens. Matter* **29** 194001
- [13] Füchsel G 2018 *J. Phys. Chem. Lett.* **9** 170–5
- [14] van der Niet M J T C *et al* 2013 *Catal. Today* **202** 105–13
- [15] Kolb M J *et al* 2016 *Phys. Rev. Lett.* **116** 136101
- [16] Lin C *et al* 2018 *Phys. Rev. Lett.* accepted (<https://journals.aps.org/prl/accepted/4007aY51X241c15909591d13a4dd51ce098ba7135>)
- [17] Thurmer K and Nie S 2013 *Proc. Natl Acad. Sci.* **110** 11757–62
- [18] Gellman A J *et al* 2017 *J. Phys.: Condens. Matter* **29** 034001
- [19] Jiang Y *et al* 2017 *J. Phys.: Condens. Matter* **29** 204001
- [20] Ortega J E *et al* 2011 *Phys. Rev. B* **83** 085411
- [21] Walsh A J *et al* 2017 *J. Vac. Sci. Technol. A* **35** 03E102
- [22] Walter A L *et al* 2015 *Nat. Commun.* **6** 8903
- [23] Janlamool J *et al* 2014 *Molecules* **19** 10845–62
- [24] Hahn C *et al* 2012 *J. Chem. Phys.* **136** 114201
- [25] Blomberg S *et al* 2017 *ACS Catal.* **7** 110–4