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D band theory

Copyright Affiliations * Corresponding Authors a Graduate School in Information Science and Technology, Hokkaido University, N-14, W-9, Sapporo 060-0814, Japan E-mail: takigawa@ist.hokudai.ac.jp Fax: +81-11-706-6470 b Precursor Research for Embryonic Science and Technology (PRESTO), Japan Science and Technology Agency (JST), 4-1-8, Honcho, Kawaguchi, Saitama 332-0012, Japan c Institute for Catalysis, Hokkaido University, N-21, W-10, Sapporo 001-0021, Japan Element Strategy Initiative for Catalysts and Batteries, Kyoto University, Katsura, Kyoto 615-8520, Japan and Department of Computational Biology and Medical Sciences, Graduate School in Border Sciences, University of Tokyo, 5-1 -5 Kashiwanoha, Kashiwa, Japan f Center for Materials Research by Information Integration, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba 305-0047, Japan g Biotechnology Research Institute for Drug Discovery , National Institute of Advanced Industrial Science and Technology , 2-4-7 Aomi Koto-ku, Tokyo 135-0064, Japan The D band metal center has been widely used to understand activity trends in catalyzed metal-surface reactions in terms of the Brønsted-Evans-Polanyi linear ratio and d-hammer-Nørskov band model. In this article, the D-band centers for eleven metals (Fe, Co, Ni, Ru, Rh, Pd, Ag, Ir, Pt, Au) and their double bimetallics for two different structures (1% doped metal or overlapping metal surfaces) are statistically predicted using machine learning methods from readily available values as descriptors for target metals (such as the density and melting enthalpy of each metal). The predictive accuracy of four regression methods with different numbers of descriptors and different set/training/test set ratios are quantitatively evaluated through statistical cross-validations. It is shown that d-band centers are reasonably well predicted by the gradient increase regression (GBR) method with only six descriptors, even when we predict 75% of the data from only 25% data for training (mean square error of average root (RMSE) < 0.5 eV). This demonstrates a potential use of machine learning methods to predict the activity trends of metal surfaces with negligible CPU time compared to the initial principle methods. You have access to this article Please wait while we upload your content... Something went wrong. Try again? Back to RSC Adv. tab navigation, 2016.6, 52587-52595 I. Takigawa, K. Shimizu, K. Tsuda and S. Takakusagi, RSC Adv., 2016, 6, 52587 If you are not the author of this article and wish to reproduce material from it in a third-party non-RSC publication, you must formally request permission using the Clearance Copyright Center. Visit our instructions for using the Release Center page of Copyright for details. Authors who contribute to CSC publications (journal articles, books or book chapters) do not need to formally request permission to reproduce material contained in this article, provided that the correct is given with the reproduced material. The reproduced material must be assigned as follows: If the material has been adapted instead of reproduced from the original publication of the Reproduced RSC can be replaced by Adapted. In all cases, Ref. XX is the XXth reference in the reference list. If you are the author of this article, you do not need to formally request permission to reproduce figures, diagrams, etc. contained in this article in third-party publications or in a thesis or dissertation, provided that correct recognition is given with the material reproduced. The reproduced material should be assigned as follows: If you are the author of this article, you still need to obtain permission to reproduce the entire article in a third-party publication, with the exception of the reproduction of the entire article in a thesis or dissertation. Information about the reproduction of rsc article material with different licenses is available on our permission requests page. Tweet Share Back to tab navigation The idea of Band D theory was introduced in the ORR section, and will be briefly discussed here. The main principle underlying the theory is that the binding energy of an adsorbate to a metallic surface is largely dependent on the electronic structure of the surface itself.⁹ For example, in the case of gaseous adsorption of hydrogen to a platinum surface, there are two primary contributions to binding energy. The first is the interaction of hydrogen state 1s with the 6s platinum band, which (according to no theory) results in the creation of a low-bonding molecular orbital (OM) and an empty anti-bonding OM. This interaction is attractive, and because the s-s coupling matrix element is not very much about transition metals, it is roughly the same for an iron or cobalt surface as for a platinum surface.⁹ Things start to get interesting, however, when we consider the interaction of the hydrogen bonding state with the metal band. The d-band metal hybridises with the orbital (σ) bonding of the adsorbate to form bonding (d- σ) and antibonding (d- σ^*) states, as illustrated below. For the metals that concern us, the state (d- σ) is full, but the extent of the filling of the state (d- σ^*) depends on the local electronic structure of the metal on the surface, that is, that of the surface. An increase in the filling of the antibonding state (d- σ^*) corresponds to a destabilization of the metal-adsorbate (and therefore weaker) interaction. As it turns out, there is an experimentally determinable parameter that correlates greatly with the extent of the filling of (d- σ^*) MO: the location of the d-band center.¹⁰ From this model it is evident that a higher D-band center (with respect to the Fermi level) corresponds to an increase in energy (in relation to the Fermi level) and subsequent decrease in state filling (d- σ^*), which means that the metal-adsorbate system is less which translates into in between metal and adsorbate. To repeat: in the context of chemisorption of molecules to a metal surface, a higher D-band center (smaller E_{dbc} - E_F) results in a stronger bond. Similarly, a lower D-band center (larger E_{dbc} - E_F) means a weaker connection. Although this argument was made for the case of hydrogen adsorption for metallic surfaces, it seems to be a reasonable model for oxygen adsorption, or any oxygen-containing species, as well.² We can now return to the question raised at the end of the ORR discussion. Platinum binds oxygen very strongly, implying that its D-band center is too high. Platinum alloy with other non-precious metals reduces the D-band center (changing the electronics and inducing a degree of irregularity in the platinum network), which in turn causes the resulting alloy to bind oxygen weaker than platinum (hence why Pt₃Ni binds very weak oxygen).¹² Thus, the alloy provides a means of adjusting the surface structure in such a way that the superpotential of orr can be minimized. Understanding the breakage and fabrication of chemical bonds on a solid surface is the starting point for any fundamental description of reactions in the solid gas or solid liquid interface. It is particularly important to understand which fundamental properties of the electronic structure of the surface determine its chemical reactivity. The News-Anderson model and the so-called D-band model proved to be particularly useful in developing such an understanding. Adsorption on a transition metal surface occurs when an atom or molecule (adsorbate) is bound in the vicinity of the surface. Depending on the strength of this bond, a share of adsorbates and metallic electrons will be involved and the energy levels of the adsorbate will be disturbed. In the News-Anderson image, the states of an electron in the adsorbate begin to interact with all states of valence on the transition metal as it approaches the surface. These metal states form an almost continuous band of states, and depending on the shape of these bands, the interaction will result in a single magnified resonance if the metal states are broad and delocalized or divided into binding and anti-binding resonances if the metal states are narrow and localized. The latter gives rise to a strong chemisorption. The figure shows an example of how the interaction energy between an adsorbate level and a semielliptic band behaves as a function of the center and width of the semi-ellipse as calculated using the News-Anderson approach. A new simplification of this approach can be made. This is the model called band D. Since all transition metals have a broadband sp that is half full, then according to the above this will lead to a single magnified resonance state. Assuming that this provides a constant contribution to the and the problem is separable so just worry about the interaction of this single resonance with d-states of each metal. Once the filling of each metal is fixed, then the variations in the binding depend only on the position of the d states in relation to the Fermi level if the d states have a smooth behavior. Since all transition metals have a wide sp band that is half full, then according to the above this will lead to a single magnified resonance state. Assuming this provides a constant contribution to the binding force and the problem is separable, then just worry about the interaction of this unique resonance with the d states of each metal. Once the filling of each metal is fixed, then the variations in the binding depend only on the position of the d states in relation to the Fermi level if the d states have a smooth behavior. Recently, we have shown for a number of different systems that adsorb with comparable electronic energy levels interact with the same surfaces in a similar way. The degeneration of energy levels now completely describes how different energies correlate and each line changes according to the structure of the surface (its reactivity). This means that we can determine the energy of a reaction of much fewer calculations. Such models of reactivity trends that highlight the important parameters that describe catalytic activity or selectivity are the essential prerequisites for the adaptation of surfaces with specified catalytic properties. We use this type of fundamental electronic structure model to analyze and predict the reactivity of metal alloys, ternary oxide surfaces, other compounds and surfaces and tense nanoparticles. Nanoparticles.

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