

Preface

Sensor arrays for chemical vapor sensing, frequently known as electronic noses, have grown in popularity over the last two decades. The relative simplicity of design and small size, leading to ease of use, make electronic noses very appealing for applications such as process control monitoring, environmental monitoring and medical diagnosis. Since the introduction of the concept of an electronic nose in the 1980s, starting with work on arrays of metal-oxide vapor sensors, there has been a significant increase in research into sensing materials and the use of arrays. Today, there are several journal articles a month discussing evaluation and selection of sensing materials as well as associated work such as transduction methods, measurement circuitry, data analysis, and sampling methods.

As approaches to designing and using sensing arrays have become more mature, and as applications of the technology have grown, it has become increasingly important to tailor the sensor materials in an array to the selected application. From the early days of research and demonstration, work has moved to focused applications, which require attention to selection of types of sensing materials as well as to selection of specific sensors within a type. Empirically derived models and first-principles computer simulations are playing an increasingly important role in our understanding of the interactions between sensing material and analytes, where the sensing materials may be polymers, metal oxides, self-assembled monolayers (SAMs), or biologically based materials.

In general, selection of sensors for a sensing array is a three-step process. First, a transduction method and a class of sensing material appropriate to that method are selected. Second, specific sensing materials within the selected class are evaluated as candidates for inclusion in the array. Third the sensing materials which will make up the array are selected. We have focused this volume on the second and third steps, selecting and evaluating specific sensing materials in order to select the elements in an array. This volume covers methods which have been used successfully in the construction of full sensing devices as well as emerging methods which show promise, with a particular emphasis on computational and statistical approaches to materials and array evaluation and selection.

We begin this volume with an introductory chapter focused on experimental methods for evaluation and development of chemical sensors and sensor arrays. Chapter 1 begins with a discussion of the mammalian model of olfaction and how it has inspired the array-based approach to chemical sensing. It goes on to establish the issues that must be considered in developing sensing materials and sensing arrays, such as sensor feature space, sensor orthogonality, geometries, and transducers. Chapter 1 also discusses the issues underlying the design of experiments and sensor evaluation, and finally, the use of experimental data in arriving at an endpoint in the evaluation process. This introductory chapter lays the groundwork for all the approaches discussed in this volume; that is, it establishes an approach to planning what to do once we have determined which sensors to test.

These computational approaches to sensor and array evaluation and selections are divided into three parts (1) First-Principles Methods of Materials Evaluation and Selection, (2) Multivariate and Statistical Methods of Materials Evaluation and Selection, and (3) Methods for Array Selection and Optimization.

Part One, Chaps. 2–6, discusses First-Principles Methods of Materials Evaluation and Selection. The general goal of developing a model of sensor performance based on first principles is not to replace existing experimental methods or knowledge-based methods of sensing material selection, but to complement these by providing quantitative approaches which can be used to prioritize the selection of new materials. First-principles design methods are being developed which can be used to plan rational modifications in the structure and function of a sensing material. This design methodology allows us to develop a theoretical understanding of the sensing material and analyte system and to predict their interactions. The predictions can then be put to an experimental test.

First-principles calculations include quantum mechanical, molecular dynamic, and structural approaches. These methods have focused primarily on developing fundamental electronic and atomic level descriptions of materials to provide insight into chemical interactions of materials with target analyte(s). Quantum mechanical techniques are discussed in Chaps. 2, 3, and 6. Molecular dynamics or atomistic techniques and statistical mechanical and multiscale approaches are discussed in Chaps. 3, 4, and 6. Chapters 3 and 6 describe a method which relies on both quantum mechanical and molecular dynamics approaches for screening sensors for their response to specific analytes. De novo structure-based design of receptors for selective chemical sensors as described in Chap. 5 applies fundamental information about structure and bonding as a basis to search for host architectures that are highly organized to form a complex with a guest molecule.

Chapter 2 uses application examples to illustrate the use of Density Functional Theory and electronic transport modeling based on nonequilibrium Green's Function in modeling carbon nanotube-based nano-electromechanical sensors and the gas-sensing properties of carbon nanotubes and metal-oxide nanowires.

Chapters 3 and 6 show that a combination of quantum mechanics with first-principles molecular dynamics can afford a great deal of information that is useful in designing and selecting materials for specific analytes.

Chapter 4 investigates the predictions of sensor responses using Grand Canonical Monte Carlo simulations. This method is used to predict the degree of sorption of analyte into polymers by calculating partition coefficients of alcohols, aromatics, ketones, esters, alkanes, and perfumes for typical gas chromatography films and compares predicted values with experimental values.

Chapter 5 presents an overview of a computer program, HostDesigner, that has been created to allow the *de novo* structure-based design of receptors that are structurally organized for complexation of small ionic and molecular guests. The methodology applies fundamental information about structure and bonding as a basis to search for host architectures that are highly organized for guest complexation.

Part Two, Chaps. 7–9, discusses Statistical and Multivariate Methods for Materials Evaluation. In this section, the work of various laboratories that have taken a combined theoretical and experimental approach to problems in vapor sensing and identification is discussed. Statistical and multivariate methods include semiempirical approaches, such as combinatorial approaches, Quantitative Structural Activity Relationships and Quantitative Structure Property Relationships, and calculation of solvation energy relationships. Many of these approaches have been developed to elucidate mechanistic aspects of sensing material activity. These approaches can, however, also be used to guide selection of materials. As array-based chemical sensing is still a relatively young field, many of the computational methods for sensor selection are still in a developmental phase.

Chapter 7 covers the experimental technique of high throughput (HT) screening, which applies combinatorial strategies to screen large sets (tens and hundreds) of sensing materials. This topic is discussed in greater detail in a companion volume in this series.

Chapter 8 discusses a statistical and multivariate method for correlating sensor response with molecular descriptors using a combination of Quantitative Structural Activity Relationships and Quantitative Structure Property Relationships. This approach develops statistically validated models of sensor response based on experimentally developed data.

Chapter 9 shows how an understanding of solubility interactions informs the selection of polymers to obtain chemical diversity in sensor arrays and obtain the maximum amount of chemical information, using principle components analysis to analyze array data. This chapter also discusses new chemometric methods which have been developed to extract chemical information from array responses in terms of solvation parameters serving as descriptors of the detected vapor.

Part Three, Chaps. 10–12, Designing Sensing Arrays, considers the computational and experimental methods that have been used together to select the components of an array designed to detect a particular analyte set.

Statistical methods based on experimental data have been used successfully to optimize an array; statistical methods may also be used with data simulated in the computational approaches discussed in Part I or with sensing data analyzed by methods discussed in Part II. The process of selecting the components of an array considers both type and identity of sensing materials, the optimum number of

sensors to be used in an array for a particular set of analytes, and how the responses of sensors will be treated in data analysis.

Chapter 10 presents a generic approach for designing sensor arrays for a given chemical sensing task. This chapter describes a correlation-based metric used to assess the analytical information obtained from chemiresistors as a function of operating temperatures and material composition combined with a statistical dimensionality-reduction algorithm to visualize the multivariate sensor response obtained from sensor arrays.

Chapter 11 discusses an iterative approach to statistical evaluation of experimental responses of candidate materials for a sensing array by developing parameters which are used to evaluate sensor performance. These three parameters are used to compute a measure of sensor suitability for inclusion in an array designed to detect a given set of analytes.

Chapter 12 discusses a hybrid sensor array, a multimodal system that incorporates several sensing elements and thus produces data that are multivariate in nature and may be significantly increased in complexity compared with data provided by single-sensor-type systems. In this chapter, various techniques for data preprocessing, feature extraction, feature selection, and modeling of sensor data are introduced and illustrated with data fusion approaches that have been implemented in applications involving data from hybrid arrays.

Finally, we close with some thoughts on future directions for work in developing computational approaches to sensor evaluation. There are several computational approaches, which have been used to design and evaluate select materials for chemical sensors. Computational methods also include use of statistical and computational approaches to characterize measured and experimentally observed analyte-sensing material interactions and sensing material responses to the presence of analyte. With the increasing use of sensing arrays, computational approaches offer complementary information to that developed through experimental approaches.

Computational Methods for Sensor Material Selection

Ryan, M.A.; Shevade, A.V.; Taylor, C.J.; Homer, M.L.;

Blanco, M.; Stetter, J.R. (Eds.)

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