Pettifor and Podloucky Respond: Phillips *et al.*[1] believe that eventually we must choose between phenomenological and microscopic treatments of structural stability. However, the two approaches perform very different but complementary roles. The *phenomenological* approach seeks to *order* the experimental data with the aid of two- (three-) dimensional structure maps. The *microscopic* approach seeks to explain the *origin* of the different structural domains within a fundamental quantum mechanical framework.

By attributing the latter role to their phenomenological models, Phillips *et al.*[1] fall between two stools —neither do they provide the best two-dimensional structural separation of the experimental data nor do they provide the correct microscopic explanation of structural stability.

Near-perfect structural separation of *all* binary compounds with a given stoichiometry A_mB_n may be made phenomenologically[2] by use of a *single* structure map (χ_A, χ_B). This is achieved by ordering of the 100 elements in the periodic table along a single axis χ so that the Mendeleev-type features are preserved. For example, groups IV*B*, V*B*, and VI*B* elements are ordered Pb, Sn, Ge, Si, Bi, Sb, As, P, Po, Te, Se, and S, so that no overlap occurs between adjacent groups. The $2p$ elements behave in a chemically distinct fashion from other elements in the same group and are assigned[2] values of χ which are free from any Mendeleev-type constraints. For example, B is inserted between Si and Bi, C between S and At. This one-dimensional ordering of the elements so that neighbors behave in a chemically not too dissimilar fashion leads to excellent *two-dimensional* structural separation for the individual stoichiometries[2] AB, AB_2, AB_3, AB_4, AB_5, AB_6, AB_{11}, AB_{12}, AB_{13}, A_2B_3, A_2B_5, A_2B_{17}, A_3B_4, A_3B_5, A_3B_7, A_4B_5, and A_6B_{23}.

On the other hand, the *three-dimensional* structure maps,[1,3] which are based on the coordinates of electronegativity, size, and valence, require sixteen separate figures to display the single stoichiometry AB—and even then the important NiAs structure type cannot be separated and is omitted.[3] This is not surprising as these coordinates violate the Mendeleev-type features of the periodic table. Firstly, Zunger's[1] s- and p-orbital *radii* show less variation in moving across a period to a neighboring group than in moving down a group. Secondly, the *electronegativity* scale assigns similar values to very different groups (e.g., IV*A* Zr, VIII Co, and III*B* Ga take[3] the values 1.70, 1.72, and 1.70, respectively). Finally, the *number* of valence electrons coordinate does not differentiate between transition metals and p-bonded elements to their right, because no distinction is made as to the angular momentum character of the orbitals. Although all these parameters or their equivalent will enter a microscopic quantum mechanical calculation, the final theoretical result must display[4] the observed Mendeleev-type characteristics, which are reflected in the single parameter χ.

Any *phenomenological* scale which produces the correct one-dimensional ordering of the elements will lead to good structural separation. However, it does not provide an explanation for the *origin* of the structural stability. For example, the fair success of Zunger's s and p core radii[1,5] in separating pd-bonded compounds should not be seen as an implication that the valence d electrons play no role in their structural stability. An explanation can only be found when we perform *microscopic* calculations which correctly handle the quantum mechanical bonding between the atoms. It then becomes apparent[4] that the angular momentum character of the valence orbitals is of prime importance as the relative stability of different building blocks is determined by whether we have sp-sp, p-d, d-d,. . . bonding. The stability of a particular type of nearest-neighbor bonding is reflected in the experimental observation[2] that the local coordination about an A atom is as a rough rule independent of the stoichiometry A_mB_n (with $m < n$).

In conclusion, we have argued that the phenomenological and microscopic approaches are complementary, not competitive. Approximate quantum mechanical schemes allow the factors determining structural stability to be investigated, but they obviously cannot produce structure maps as accurate as the experimental data itself. However, besides their pedagogical value, microscopic schemes are becoming increasingly important for predicting metastable phases, the structure of grain boundaries, etc., because these are not readily accessible to experiment and hence amenable to phenomenological interpolation.

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