The Hitchhiker’s Guide to the Periodic Table: Which Superhard Inorganic Compounds Are Missing the Market?

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It is often asserted that the hardest substance with ten points on the Mohs scale is diamond. However, the most interesting features of the present day require the discovery of new superhard materials. The first thing that needs to be done is to predict properties of 40,000 hypothetical compounds using modeling principles of solid mechanics and crystal chemistry. The list of these properties, not exhaustive, include bulk modulus, shear modulus, elastic modulus, melting and boiling points, and solubility. In this investigation microscopic properties (ionic radii, structure, electronegativity) were linked to aforementioned macroscopic mechanical properties. Using optimization calculus, the desired values for atomic-scale properties were determined and compared to those of a selected group. After minimal standards for a compound to be considered a superhard one have been set, the list has been narrowed down and additional filters of selection (melting temperature, solubility, costs per unit, and safety measures according to National Fire Protection Association) were applied. From this research it can be seen that top 10 materials with their potential application were found. Although the model was designed for ionic compounds, the adjustments made allowed to predict the properties for covalent compounds, where uncertainty, depending on a structural type, varies of about 10 percent. I have shown that inorganic materials of comparable hardness to that of diamond exist, and proposed that their use must find place in the production of locksmith, grinders, surgical equipment, military and bomb-defusing equipment. Hopefully, the results clearly point to the need for further study.