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A new Virtual Crystal Approximation approach ROBERTA POLONI, ICMAB-CSIC, Campus UAB E-08193 Bellaterra, Barcelona (SPain), JORGE IÑIGUEZ, ALBERTO GARCIA, ENRIC CANADELL, ICMAB-CSIC, Campus UAB E-08193 Bellaterra, Barcelona (Spain) — It is well known that the virtual crystal approximation (VCA) provides an efficient method for studying disordered alloys and solid solutions by first-principles. Although several studies have reported VCA results regarding stability issues by using energetic considerations, here we propose a new approach based on alternative structural indicators. The reason for this is that it is still not clear whether energy comparisons for different virtual compositions are trustworthy. Our non-fully-predictive scheme makes use of some experimental information in order address structural problems like atomic ordering and/or partial occupation at some site. We look at different figures of merit (energy derivatives), depending on the amount of experimental information taken into account, and we minimize them with respect to different possible structural configurations. By applying our approach to a wide number of well known systems (oxinitrides, borocarbides, perovskites, etc.) we have been able to reproduce the experimental structure in all cases.

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