# Article information:

First principles impurity diffusion coefficients — Penn State  
<https://pennstate.pure.elsevier.com/en/publications/first-principles-impurity-diffusion-coefficients>

# Article summary:

1. This article reports the prediction of impurity diffusion coefficients entirely from first principles, using density-functional theory (DFT) calculations.

2. The results show excellent agreement with experimental data and discuss the factors contributing to the trends in diffusivities of these impurities.

3. The article specifically calculates the impurity diffusion coefficients of Mg, Si and Cu in dilute face-centered cubic Al alloys.

# Article rating:

May be slightly imbalanced: The article presents the information in a generally reliable way, but there are minor points of consideration that could be explored further or claims that are not fully backed by appropriate evidence. Some perspectives may also be omitted, and you are encouraged to use the research topics section to explore the topic further.

# Article analysis:

The article is reliable and trustworthy as it provides a detailed explanation of its methodology and results, which are backed up by experimental data. Furthermore, the authors provide an in-depth discussion on the factors contributing to the trends in diffusivities of these impurities, which adds to its credibility.

However, there are some potential biases that should be noted. For example, the authors only consider three specific impurities (Mg, Si and Cu) in their calculations, which may not be representative of all possible impurities that could be present in such alloys. Additionally, they do not explore any counterarguments or alternative explanations for their findings.

In conclusion, this article is generally reliable and trustworthy but should be read with caution due to potential biases mentioned above.

# Topics for further research:

* Diffusivity of impurities in alloys
* Factors affecting diffusivity of impurities
* Alternative explanations for diffusivity trends
* Impurity diffusion in alloys
* Counterarguments to diffusivity trends
* Impurity diffusion in metals

# Report location:

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