

# Role of surface chemistry in Safe-by-Design



Control over the physical dimensions of 2-D NMs (size, shape and layer number) is very difficult, so these parameters are not simple to vary during Safe-by-Design (SbD). This leaves the control of the surface chemistry as the most viable approach towards SbD for this family of NMs. This factsheet summarises how introduction of surface functionality to graphene oxide can change the potential for both hazard and exposure to humans and the environment.

## Deciding a surface modifier and modification strategy

### Requirements for a surface modifier:

- Proven biocompatibility
- Compatibility with ENMs' properties
- Stability in formulation
- Chemical suitability
- Low cost
- Applicability

### Factors influencing NM toxicity:

- Size/dimensions
- Dissolution
- Chemical nature/chemistry of surface
- Aggregation

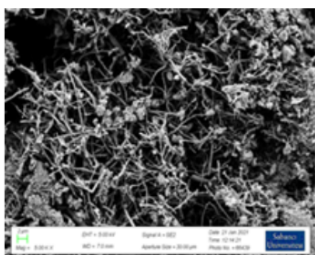
### Modification Strategies

- Surface properties of NMs
  - Defined by the synthesis procedure
  - Impurities remained on NM surface
  - Agglomeration/Aggregation
  - Chemical attachment of modifier directly
- Complete coating with a polymer, etc.

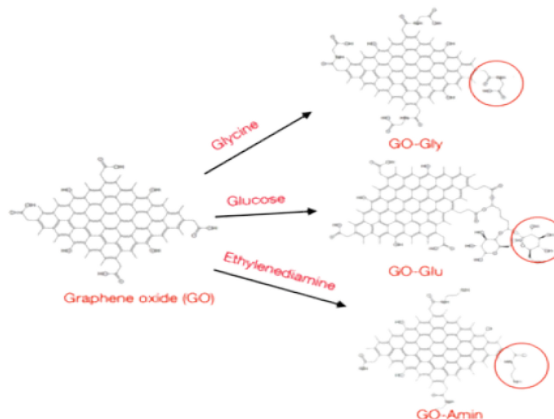
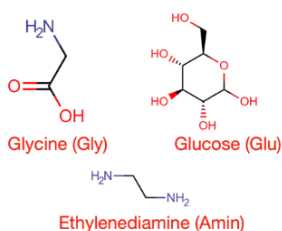
### Practical implementation

The SbD4Nano project has demonstrated how functionalisation can impact multiple physicochemical parameters and these do not always change risk in the same direction.

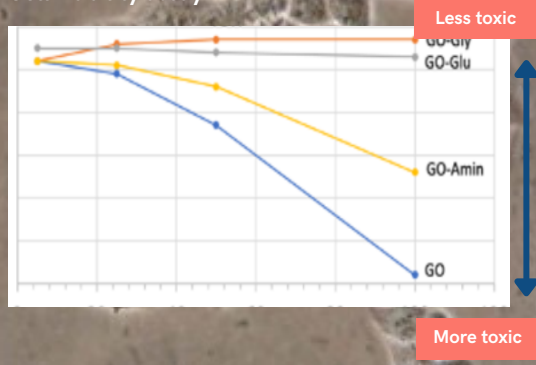
Test substance:  
carbon nanofibers, graphene, graphene oxide (GO)



Surface Modifiers



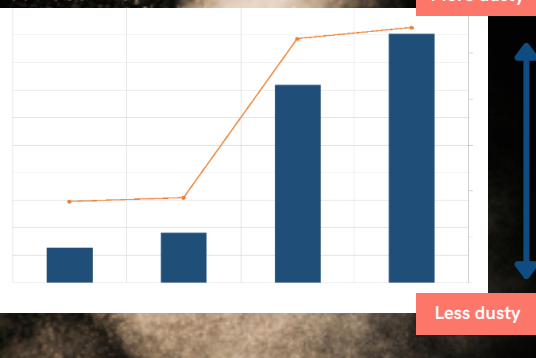
### Cell viability assay



### Algae growth inhibition assay



### Dustiness Index and Specific Surface Area



### SbD4Nano tools

The e-infrastructure contains a decision support tool that guides users to choose the best surface functionalisation options. The project has developed a screening approach to predict functionalised NM properties from those of the functionalising substance.

### Conclusion

As the interface to the biosystems, altering surface chemistry of NMs can serve an effective strategy for SbD implementation into safer nanomaterials. Each NM case should be evaluated to decide the surface chemistry and modifications strategy.

