

Methodology

Literature data

Ce-doped BG

Literature data

Co-doped BG

Hyperparameter

Tuning

Leveraging machine learning for the determination of optimal cerium and cobalt content

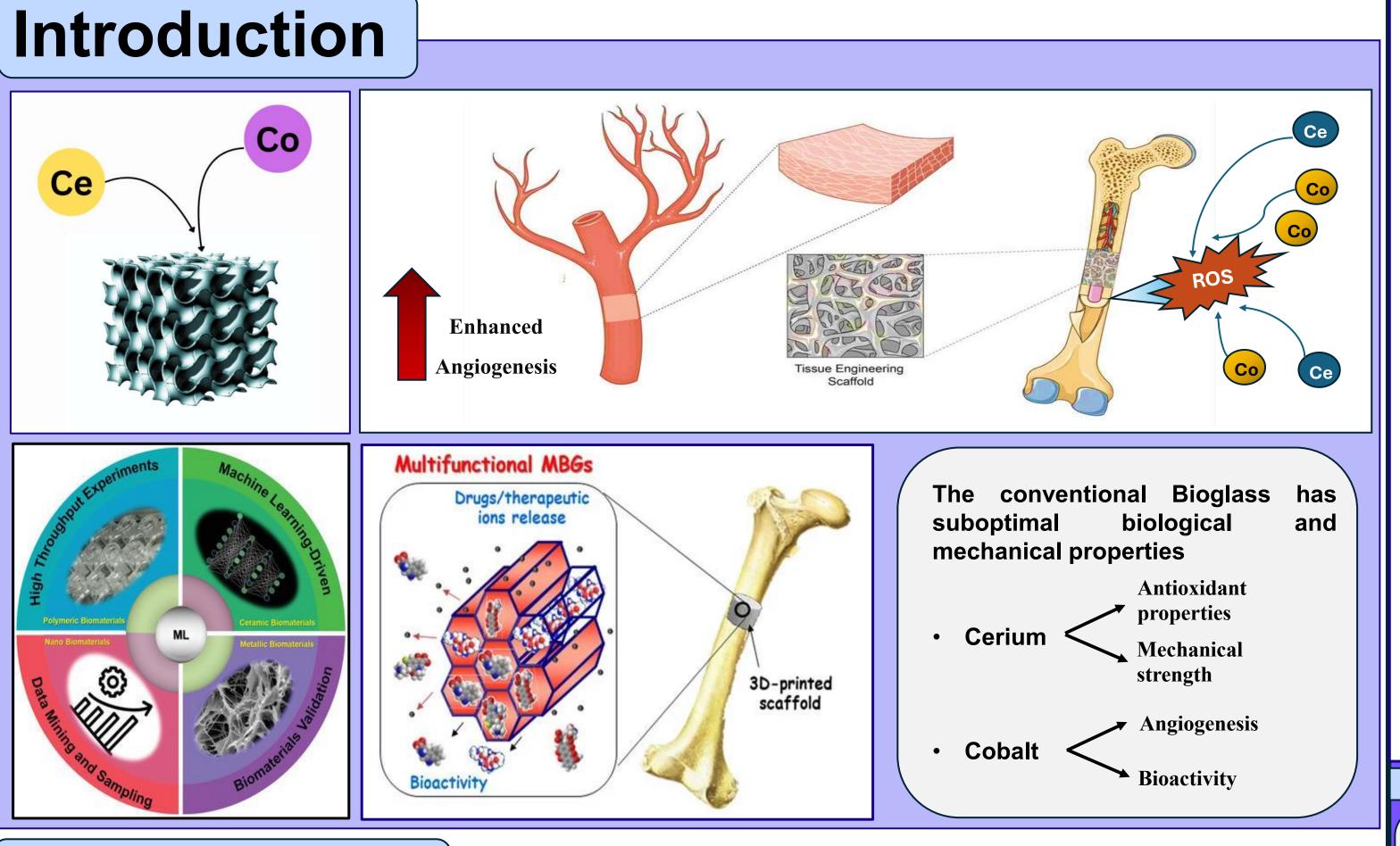
in bioglass scaffold for improved angiogenesis and mechanical properties

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KDE Plot - Cell Viability 4



Study Workflow Diagram

Catboost

Biological + Mechanical

Properties

Collection

of Dataset

Data

Preprocessing

ML Model

Training

Adaboost

 B_2O_3

CaO

XGB

Regressor

Evaluation

Composition

Prediction

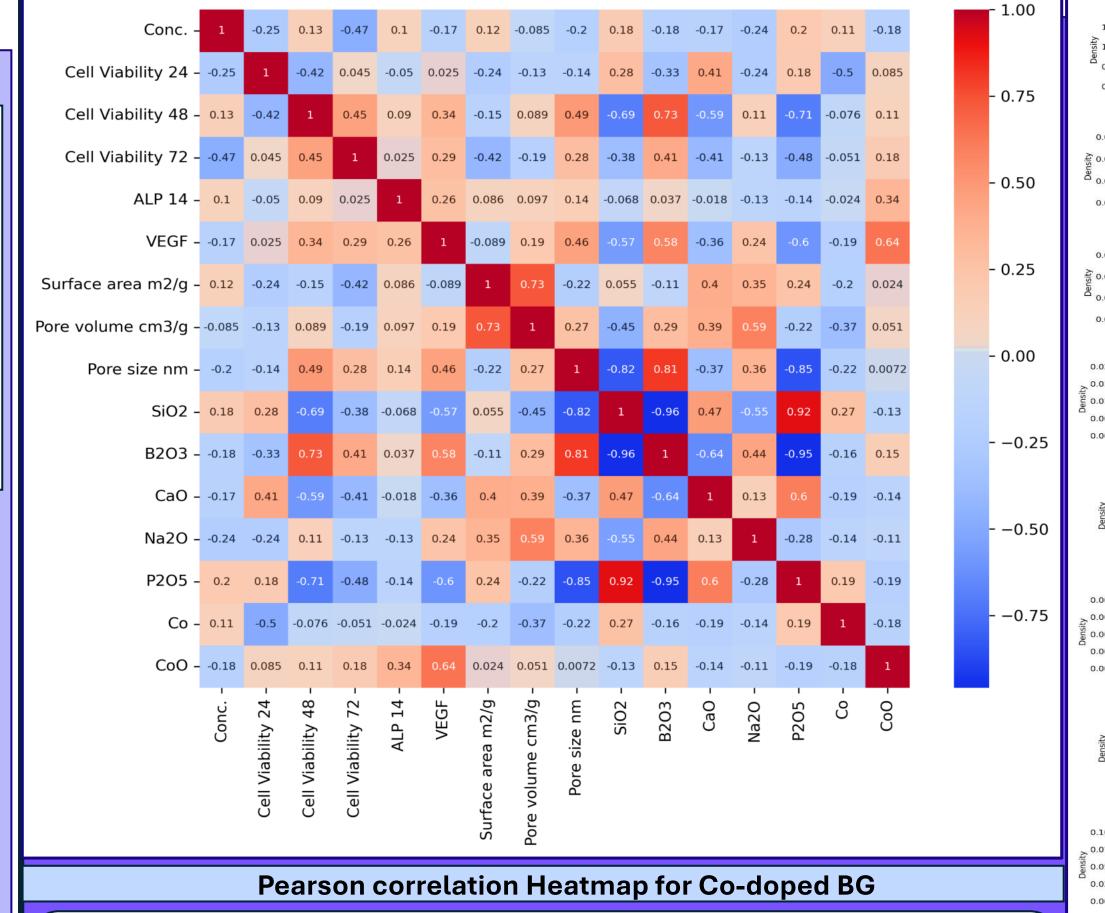
Material

Development

Gaussian

Process

Regressor



➤ Showed interesting inferences for the high correlation of B₂O₃ and CoO

- with VEGF. Higher pore size relates to higher VEGF and cell viability.
- Surface area can be seen as inversely proportional to cell viability.

KDE Plot - Pore size nm KDE Plot - VEGF 0.6 -**KDE plots Co-doped BG**

Dopants and Models Summary SHAP Summary Plot for CeO2 SHAP Summary Plot for CoO 4-4---ALP 7d Pore size nm Surface area m2/g Surface area m2/g Cell Viability 72 Cell Viability 24h Cell Viability 24 Pore size nm Pore volume cm3/g Cell Viability 72h Cell Viability 48 Cell Viability 48h Cell Viability 96h Conc. Pore volume cm3/g -1.0 -0.5 0.0 0.5 1.0 1.5 2.0 SHAP value (impact on model output) SHAP value (impact on model output) SHAP Analysis- Co-doped BG

SHAP Analysis- Ce-doped BG Ce-doped BG Co-doped BG Gaussian Process Regressor 0.72 XGB Regressor N2 -AdaBoost 0.78 Extra Tree Regressor CatBoost 0.83 Random Forest Regressor 0.81 K Neighbours Regressor 0.82 8.0 R² scores Model-wise performance comparison The resulting composition obtained can be used to

develop application-specific materials with enhanced

The models trained were used to predict 2 samples with the following mechanical and biological features and the composition obtained are: Sample 1 (Ce) Sample 2 (Co) **Properties** Conc. 8.0 0.8 **Cell Viability 24h** 93 89

Cell Viability 48h

Cell Viability 72h

Cell Viability 96h	82	1.12
ALP 7d	1.2	1.3
Surface area m ₂ /g	225	225
Pore volume cm ₃ /g	0.3	0.35
Pore size nm	2	2.2
Composition(mol %) Sample 1 (Ce)	Sample 2 (Co)
SiO ₂	64.4	69
CaO	23.33	27.4
Na ₂ O	5.07	0
P_2O_5	4.3	5
CeO ₂	2.9	0
CoO	0	3.6

Results and Discussion

Extra Tree

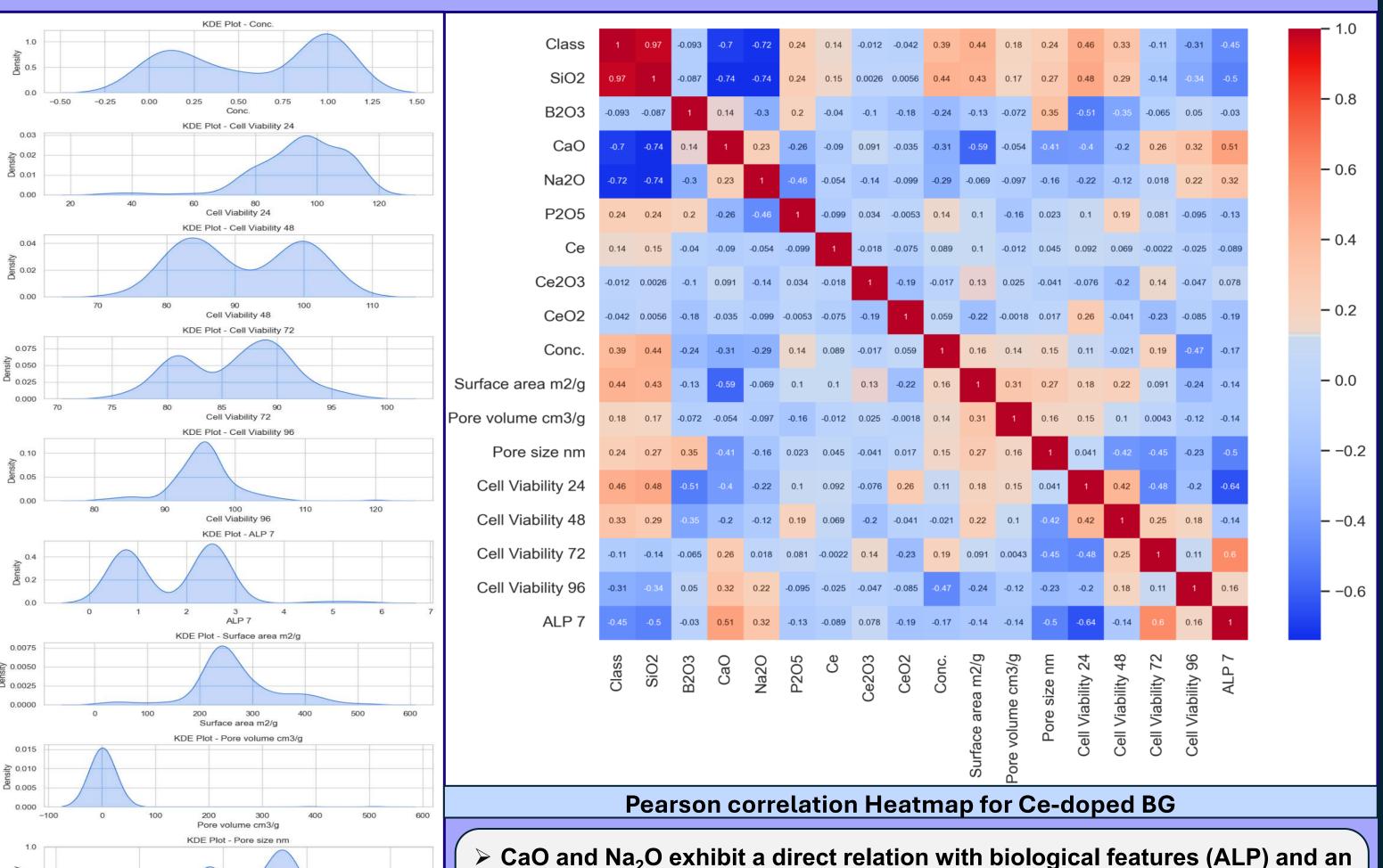
Regressor

K Neighbors

Regressor

Na₂O

Distribution of Features & Targets present in the Dataset



inverse relation with surface area and pore size.

➤ CeO₂ also shows an inverse relation with surface area.

B₂O₃ content relates directly to pore size.

Conclusion

mechanical and biological features.

- > Important variations in Ce or Co-doped BG activity on biological properties like cell viability, VEGF secretion, and ALP are mainly linked to the composition of BG and, in particular, to their content of Ce and Co ions.
- > The performance of a Regression type ML model depends on its R² Score and RMSE.
- > Extra Tree Regressor Model performed the best for Ce-doped BG and AdaBoost performed the best among all the models trained for Co-doped BG with an R² Score of 0.84 and 0.78 respectively.
- > The trained model can now give the composition of Bioglass with Ce and Co of desired properties.

Future Scope

- > Assess the material compositions predicted by the ML model by comparing them with original samples and evaluating their biological and mechanical properties.
- > Integrate the current developed model with antibacterial properties in future studies.
- Aim to develop a multifunctional material based on Bioglass by combining biological, mechanical, and antibacterial properties.

Acknowledgement

References

- Supervisor Prof. Kantesh Balani
- **Project Mentor Murli Manohar**
- ✓ Head, MSE Department
- **✓ All the staff of the Library, MSE Department**
- Staff and Colleagues of BPCL Lab
- ✓ M.M. Echezarreta-Lopez et al. International Journal of Pharmaceutics (2013)
- ✓ María Vallet-Regí et al. Pharmaceutics (2022)
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KDE plots Ce-doped BG



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