Artificial Neural Networks – Applications in Modeling Physical and Chemical Processes

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Artificial Neural Networks (ANNs)

- High speed mathematical models
- Black-box models – do not require any explicit mathematical expression
- Describe the investigated phenomena based on the input-output relationship
- Can solve linear & non linear multivariate regression problems
- Capacity to solve problems such as:
  - Classification
  - Identifications
  - Pattern recognition
  - System control
  - Prediction

❖ Jin, C.; Wang, G.; Le, A.-T.; Lin, C. D., *Sci. Rep.*, **2014**, *4*, 7067
❖ Neocleous, C.; Schizas, C., *Methods and Applications of Artificial Intelligence, SETN 2002, Lecture Notes in Computer Science*; **2002**, Vol. 2308, 300–313
❖ Maleki, N.; Kashanian, S.; Maleki, E.; Nazari, M., *Biochem. Eng. J.*, **2017**, *128*, 1–11

ANNs - Applications

- Medicine
- Food technology
- Engineering
- Physics
- Chemistry

- Bhatikar, S. R.; DeGroff, C.; Mahajan, R. L., *Artif. Intell. Med.*, **2005**, *33*, 251–260
- Chen, Z.; Ma, W.; Wei, K.; Wu, J.; Li, S.; Xie, K.; Lv, G., *Appl. Therm. Eng.*, **2017**, *112*, 226–236
- Oladunjoye, A. O.; Oyewole, S. A.; Singh, S.; Ijabadeniyi, O. A, *LWT - Food Sci. Technol.*, **2017**, *76*, 9–17
- Gherman, A. M. M.; Tosa, N.; Cristea, M. V.; Tosa, V.; Porav, S., *Mater. Reserch Express* **2018**, *5*

ANNs - Topology

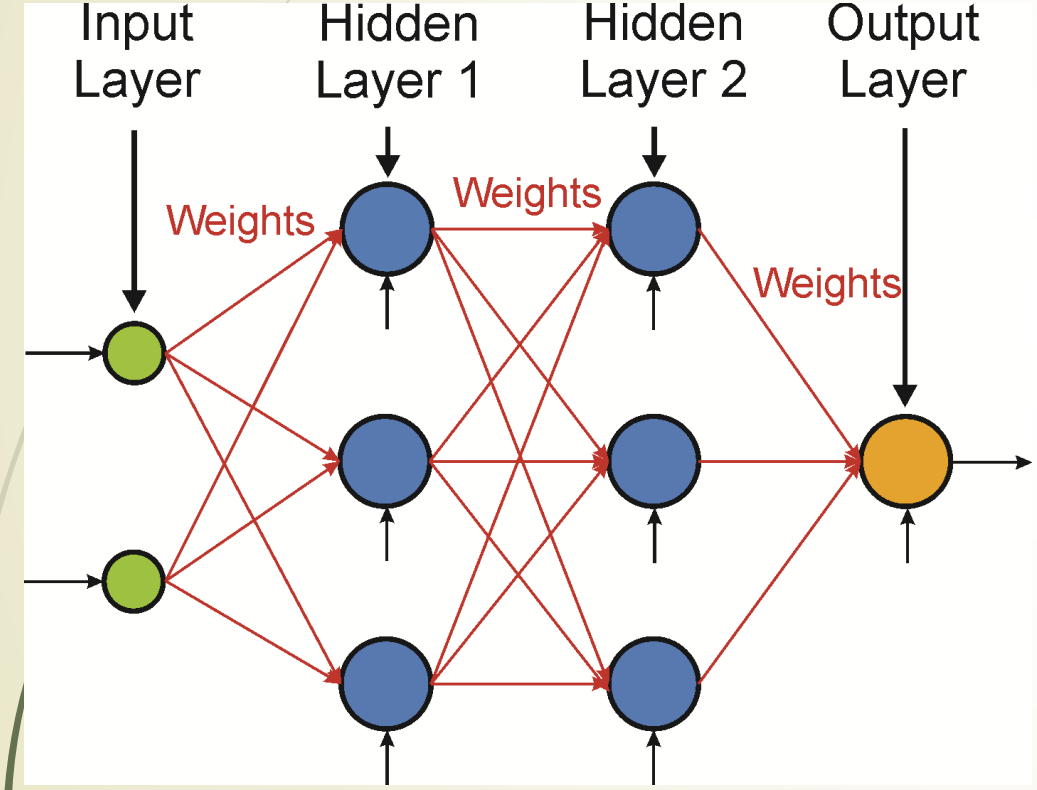


Fig1. ANN Architecture

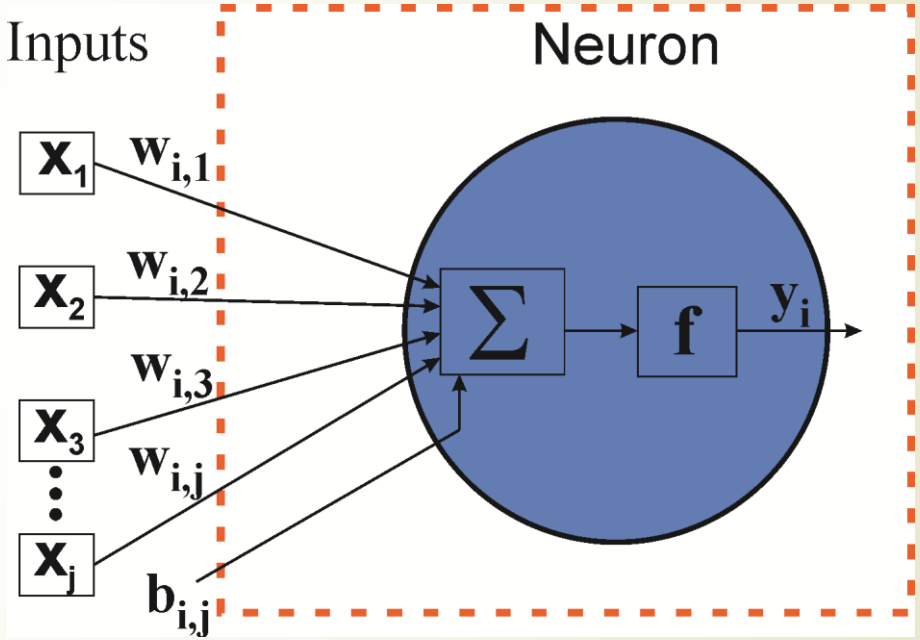


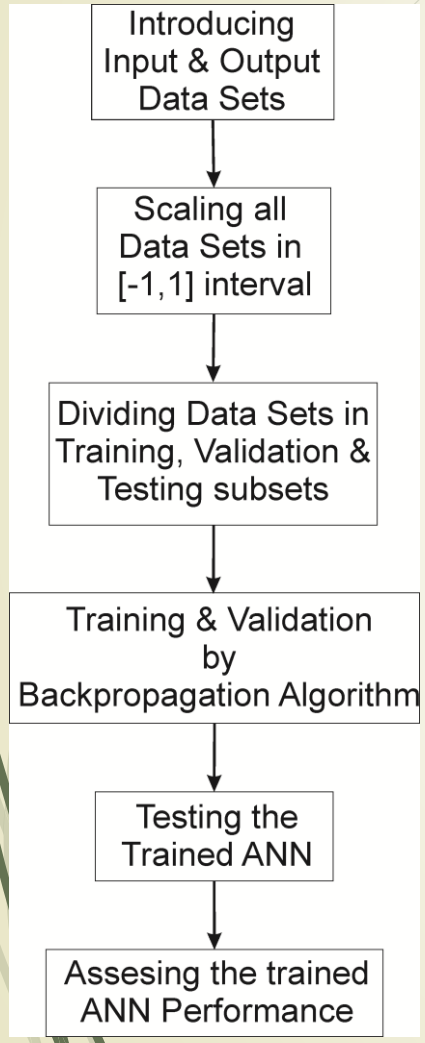
Fig2. Schematic representation of a neuron

❖ Hagan, M. T.; Demuth, H. B.; Beale, M. H.; De Jesús, O. *Neural Network Design (2nd Edition)*; 2014; ISBN 9780971732100.

Aim

- Exploit ANN capabilities to:
  - Model of the AuNPs photochemical generation process (ANN 1)
    - Determine the gold nanoparticles (AuNPs) size
  - Predict the output of a high-order harmonic generation (HHG) process (ANN 2)
    - Predict the Harmonic yield

General Features



- Modifies the weights and biases starting from the output ➡ input to minimize the network error

- Pearson Correlation Factor
- Relative Error

Aim - ANN 1

- Model of the AuNPs photochemical generation process (ANN 1)
  - Determine the gold nanoparticles (AuNPs) size
  - Evaluate the influence of each process parameter on the AuNPs size

ANN1 - Motivation

- AuNP size – essential for AuNPs application
- AuNPs size – experimentally determined with TEM only after synthesis
- Important to know the AuNPs size before beginning the synthesis
- There is NO mathematical model that
  - considers all parameters that influence the AuNPs generation

ANN 1 - Performance

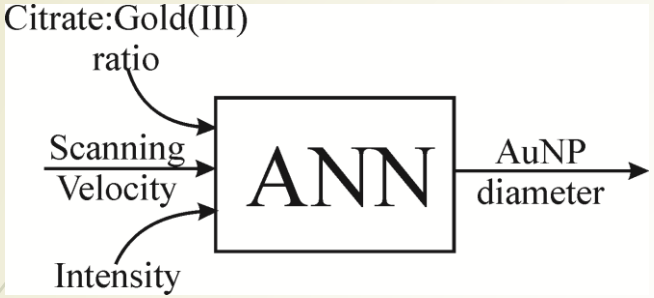


Fig3. Schematic representations of the ANN

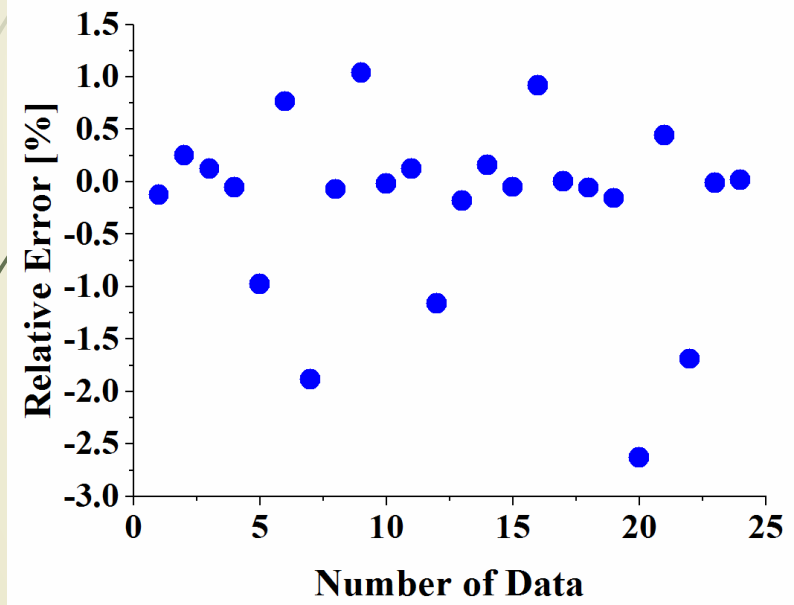


Fig4. ANN I – Testing Data - Relative Error

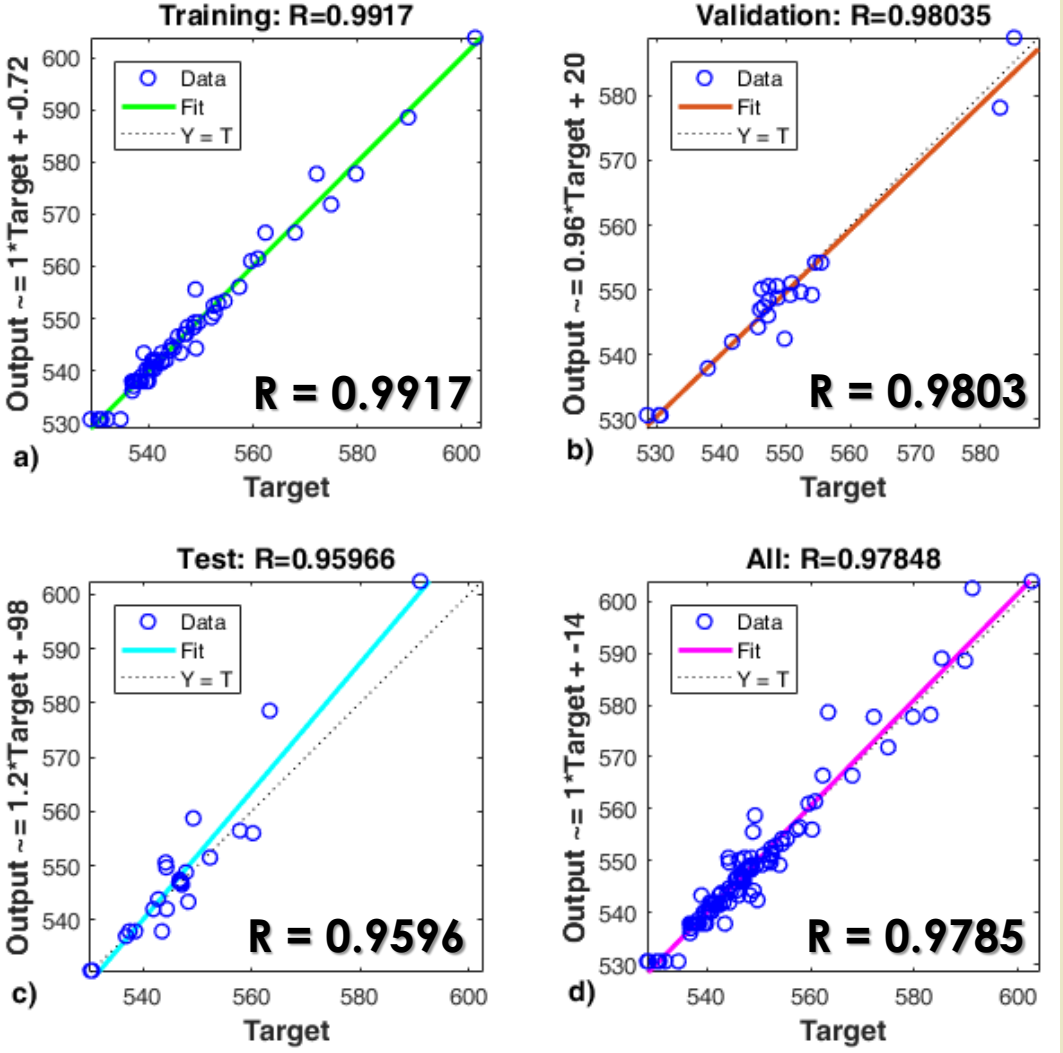


Fig5. ANN I – The Pearson correlation factor

- High Pearson Coefficients, Low Relative Errors ➡ The ANN can reliably predict the AuNPs size

A. M. M. Gherman, N. Tosa*, M. V. Cristea, V. Tosa, S. Porav and P. S. Agachi, Materials Research Express, 5 (2018), 085011, 1-13.

ANN1 model Predictions - The influence of process parameters on the AuNPs size

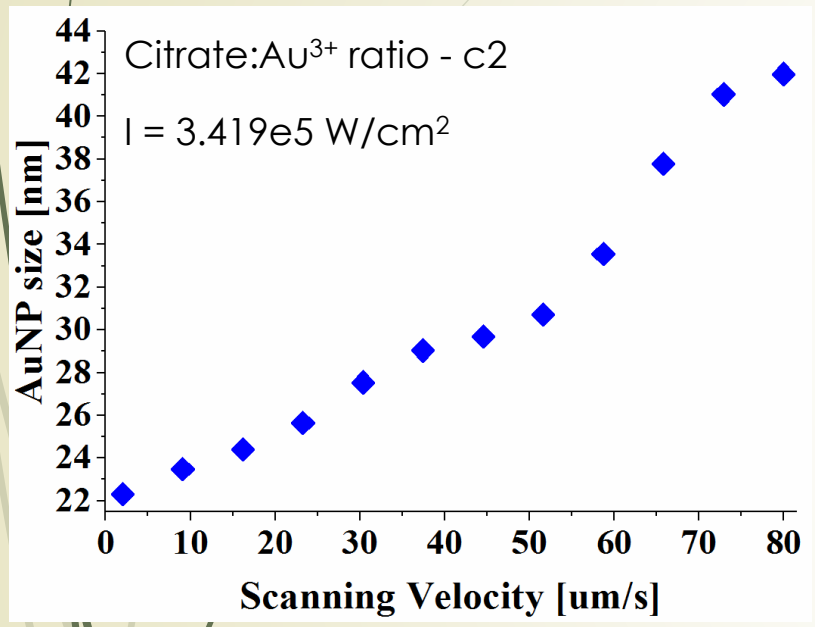


Fig6. Influence of scanning velocity on AuNP size

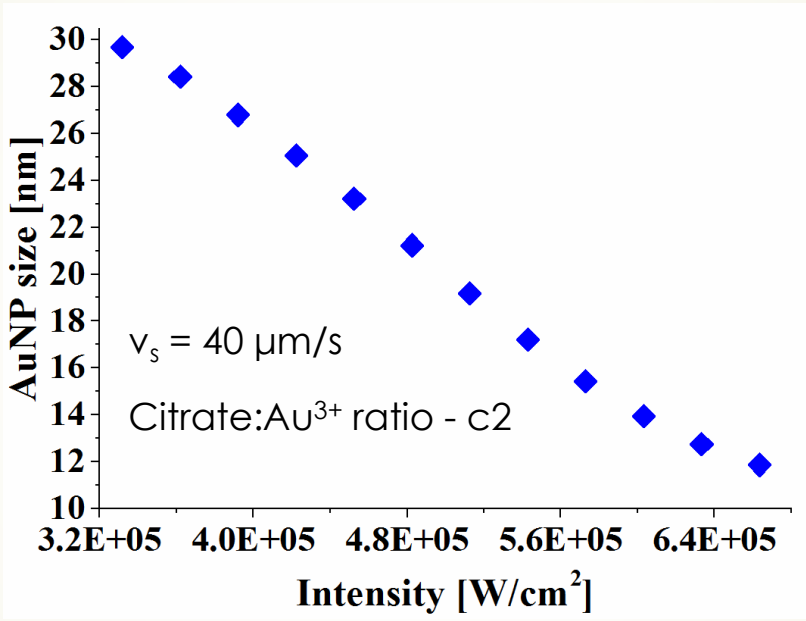


Fig7. Influence of Intensity on AuNP size

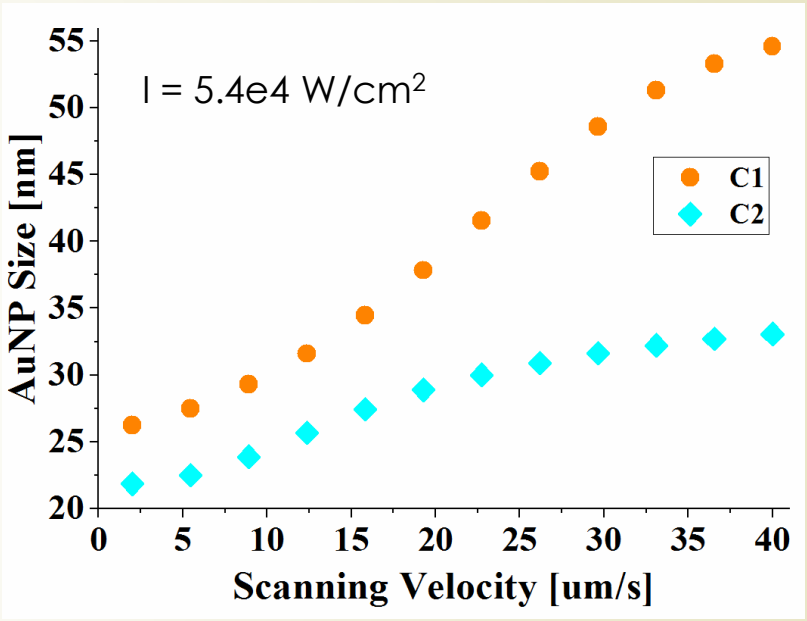


Fig8. Trend in AuNP size when citrate:Au3+ ratio changes

↑ Scanning Velocity → ↑ AuNPs Diameter

↑ Radiation Intensity → ↓ AuNPs Diameter

↑ Citrate:Au3+ ratio → ↓ AuNPs Diameter

A. M. M. Gherman, N. Tosa*, M. V. Cristea, V. Tosa, S. Porav and P. S. Agachi, Materials Research Express, 5 (2018), 085011, 1-13.

Conclusions

- Developed ANN is capable to reliably predict the AuNPs dimension
  - Determined that:
    - AuNPs size increases with the increase of the scanning velocity
    - AuNPs size increases with decrease in the radiation intensity
    - higher citrate:Au^{3+} ratios lead to smaller AuNPs

Aim – ANN 2

- Predict the output of a high-order harmonic generation (HHG) process (ANN 2)
  - Predict the Harmonic yield

ANN 2 - Motivation

- HHG – experimental technique for obtaining coherent radiation in the XUV to soft X-ray spectral domain (1-100 nm) on the attosecond timescale (1 as $=10^{-18}$ s)
- HHG process
  - Highly nonlinear interaction between a strong laser pulse and an atom
  - Has low efficiency ($\sim 10^{-5}$)
- **For experiments ➡ Crucial** to **find the optimum photon flux** obtained within a restricted parameter space
- Optimum photon flux obtained
  - **Experimentally** - scan along many tunable parameters ➡ **time-resource consuming**
  - **Simulation - 3D model ➡ Computational effort** – very difficult to be managed

ANN 2 – Performance

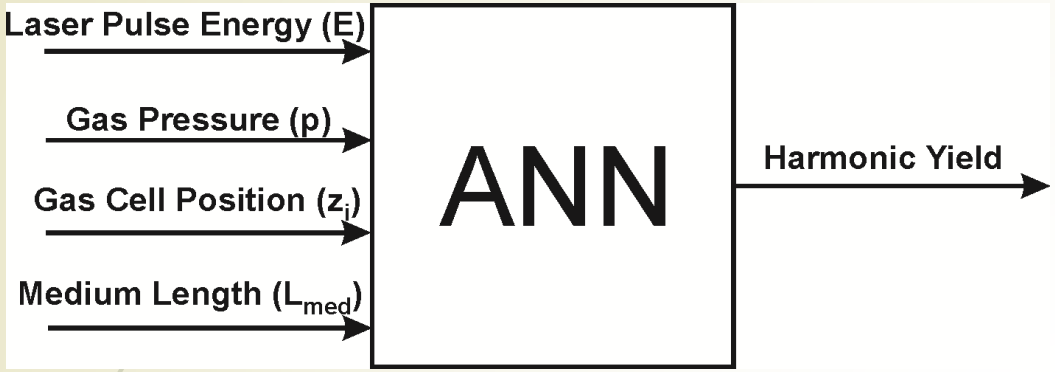


Fig10. Schematic representations of ANN 2

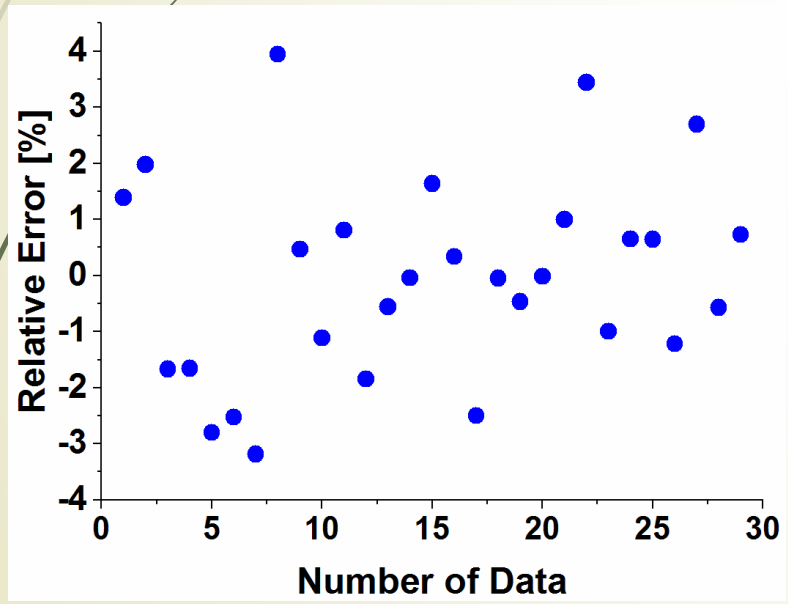


Fig11. ANN I – Testing Data - Relative Error

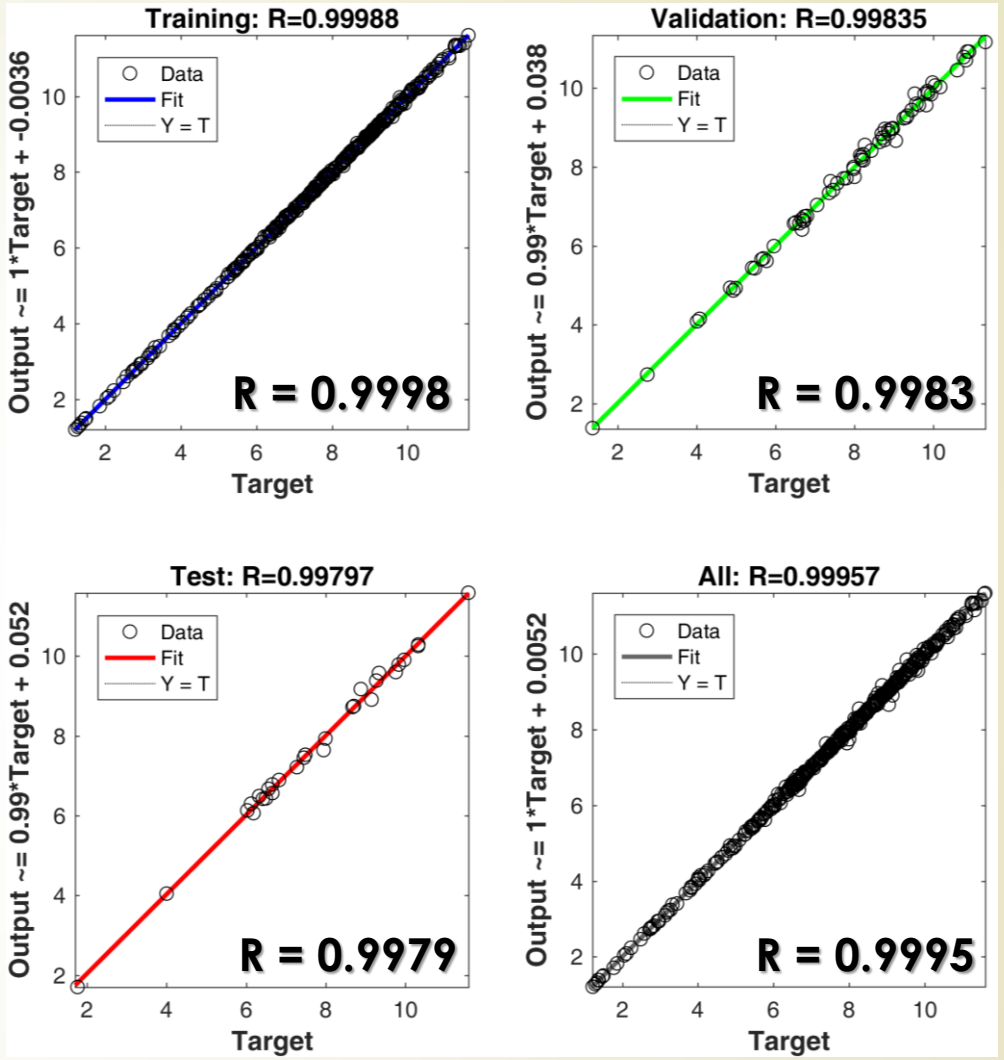


Fig12. ANN I – The Pearson correlation factor

- High Pearson Coefficients, Low Relative Errors

A. M. M. Gherman, K. Kovacs *, M. V. Cristea, V. Tosa, Artificial Neural Network Trained to Predict High-harmonic Flux, Submitted Article

ANN 2 - Model Predictions

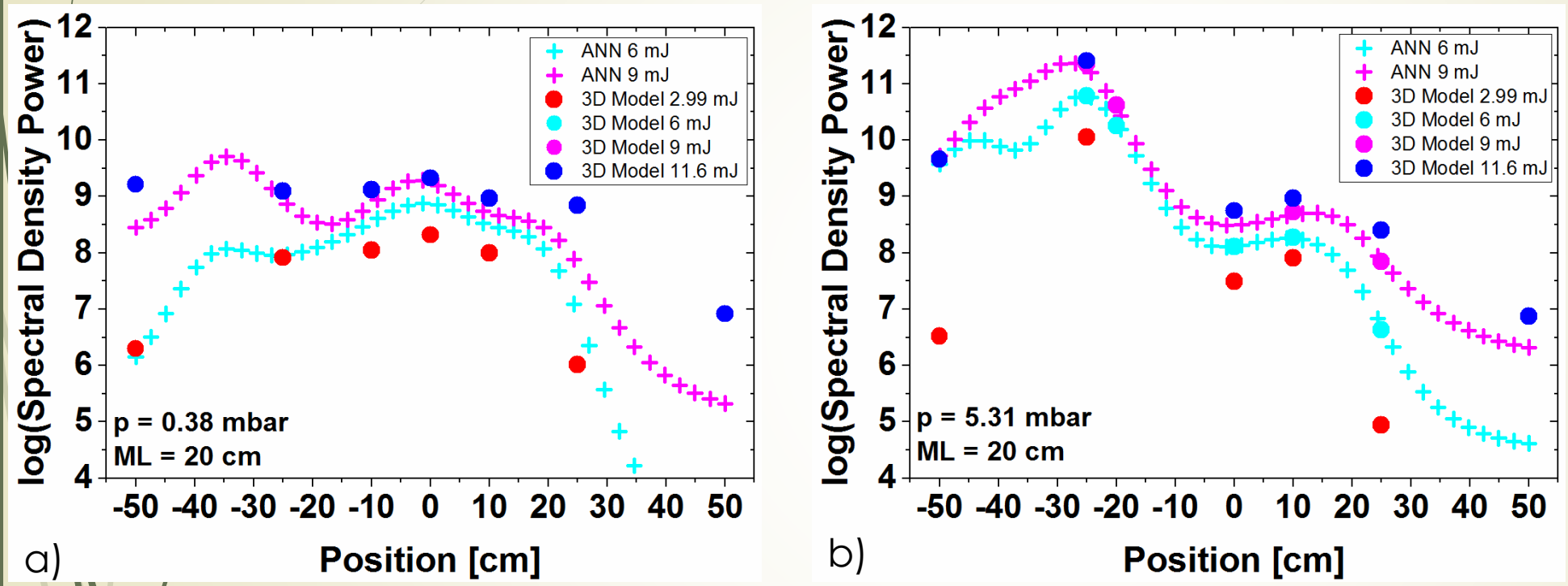


Fig13. Harmonic Yield vs Gas Cell Position

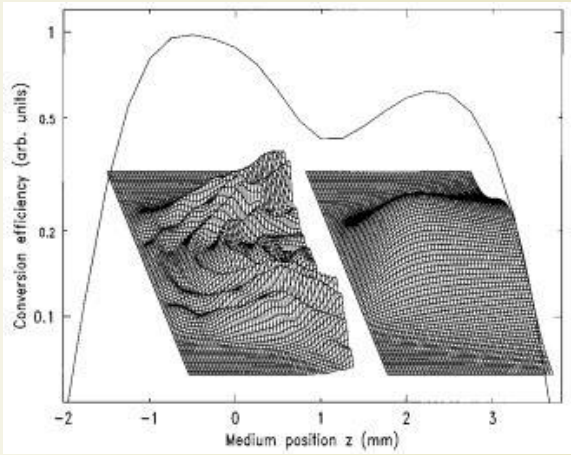


Fig14. Conversion efficiency vs Position (Balcou)

- ANN prediction - Captures the highly nonlinear dependence of the harmonic yield on gas cell position
- Trained ANN - Able to reproduce the transition between different conditions for HHG

- A. M. M. Gherman, K. Kovacs *, M. V. Cristea, V. Tosa, Applied Sciences, Submitted Article
- A. Balcou, P.; Salieres, P.; L'Huillier, A.; Lewenstein, M., *Phys. Rev. A* 1997, *55*, 3204–3210,

ANN 2 - Model Predictions

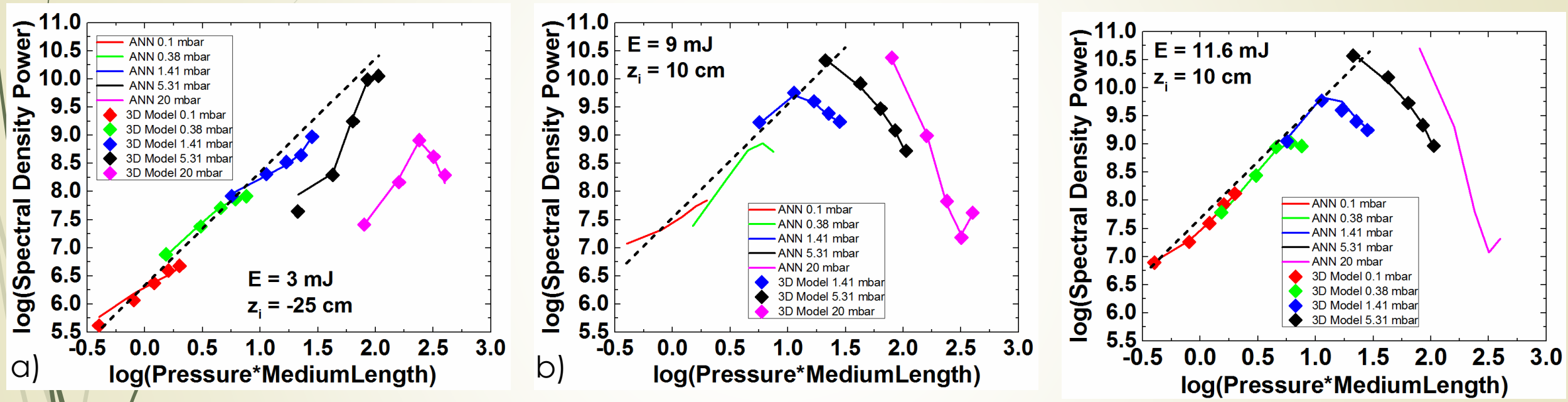


Fig14. Harmonic Yield vs Optical density of the medium

- ANN - reliably predicts quadratic growth of the yield in the low density regime
- E = 11.6 mJ – for the high density regime, ANN predictions follow a similar trend as the one obtained with the 3D model for smaller energies

A. M. M. Gherman, k. Kovacs *, M. V. Cristea, V. Tosa, Applied Sciences, Submitted Article

Conclusions

- Trained ANN
  - Has excellent performances ➡ Can reliably predict the HY
  - Captures the highly nonlinear dependence of the harmonic yield on gas cell position
  - Able to reproduce the transition between different physical conditions for HHG
  - Predicts quadratic growth of the yield in the low density regime
  - Offers a quick help in designing new experiments

General Conclusions

- **A fast and easy method was developed to determine the AuNPs size before synthesizing the NPs**
- **The influence of each process parameter on the AuNPs size was determined**
- **A fast and reliable method was developed to predict the outcome of a HHG experiment in the unexplored parts of the multi-dimensional parameter space**

- **Acknowledgement**
  - This work was supported by a grant of the Romanian Ministry of Research and Innovation, project code PN 18 03 02 01, within Core Program


Thank you for your attention!