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Mesoporous silica thin films containing propyl-copper-phosphonate units inside vertically aligned pores as a novel material with tunable nonlinear optical (NLO) properties.

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In this work we propose the compound based on porous silica matrix containing polar functional units to use as a material for desirable second and third order nonlinear optics (NLO) properties. As a matrix we postulate mesoporous silica in the form of thin films, having 2D hexagonally ordered pores with diameter about 2 nm, aligned perpendicularly to the substrate. This material plays a role of neutral (non-polar) matrix for active polar units. One of a crucial feature of our matrix is its transparency in the visible spectral range which allows the functional groups that are inside the material to be excited efficiently. As an optically active centres we propose copper propyl phosphonate units that are polar - bounding between copper and oxygen atoms at the phosphonate units have polarized covalent character. Such copper-containing functional groups are regularly distributed and anchored inside silica matrix. By modification of functional groups concentration inside the matrix we are able to tune degree of supramolecular interactions and also charge distribution in functional groups. Therefore modification of functional groups content can be used for tuning the NLO susceptibilities. Nevertheless, modification of functional groups content can result in systems reorganization, what can lead to quasi phase transition. For this reason it is a vital task to investigate this phenomenon in details, to be able to take it into account during NLO properties tuning.

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